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AUTHOR INDEX, 1978

- Abbot, John, 880-4
 Adams, David M., 776-82, 782-8
 Aime, Silvio, 534-40
 Airoldi, Claudio, 1102-4
 Albano, Vincenzo G., 459-63, 463-7
 Alcock, Nathaniel W., 394-9, 638-46, 1282-8, 1324-8
 Alcock, Roland M., 115-23, 123-31
 Allen, Christopher W., 173-7
 Al-Ohal, Abdul Razzak, 889-95
 Al Omer, Sabah S., 1589-93
 Andersen, Richard A., 446-53
 Andreocci, Marco, 695-8
 Angus, Philip C., 938-43
 Anichini, Andrea, 577-83
 Annibale, Giuliano, 728-34
 Arena, Giuseppe, 1090-4
 Ashworth, Terence V., 340-7, 1032-6, 1036-9, 1040-2, 1043-6
 Askalani, Pakinam, 996-1000, 1001-8
 Asperger, Smiljko, 500-2
 Atwood, Jerry L., 1189-95, 1573-6
 Aymonino, Pedro J., 1603-6
 Azam, Kazi A., 1201-6
 Azeez, Wissam I., 677-80
 Baertschi, Peter, 496-500
 Bagnall, Kenneth W., 295-8, 638-46
 Bailey, Pamela M., 1825-30
 Baker, Edward N., 416-18
 Bamford, Clement H., 4-8
 Bandoli, Giuliano, 373-80
 Barbucci, Rolando, 1090-4
 Barker, Geoffrey K., 734-40, 1839-47
 Barnett, George H., 587-92
 Barrer, Richard M., 598-601, 1746-52
 Barton, Trevor J., 608-11
 Battaglia, Luigi P., 583-7
 Beck, Wolfgang, 1155-60
 Begley, Michael J., 1094-8
 Bellachioma, Gianfranco, 695-8
 Bellerby, John, 1185-9
 Bellitto, Carlo, 1207-12
 Benfield, Robert E., 1554-68
 Bennett, Ross, 1046-51
 Benson, Ian B., 1240-6
 Bernal, Ivan, 1189-95, 1664-70
 Berthon, Guy, 1433-8
 Bertini, Ivano, 1269-73
 Bied-Charreton, Claude, 1807-13
 Birchall, John D., 604-7
 Bishop, Edward O., 1654-8
 Bishop, Michael W., 1654-8
 Blacklaws, Isobel M., 753-8, 877-9
 Blake, Antony B., 868-71
 Blandamer, Michael J., 244-7, 996-1000, 1001-8, 1086-90
 Blesa, Miguel A., 1603-6
 Boese, Roland, 1387-92
 Boeyens, Jan C. A., 1438-44
 Bombieri, Gabriella, 677-80
 Bone, Stephen P., 1544-8
 Bonny, Alan, 506-11, 722-6, 938-43, 1569-73
 Boorman, P. Michael, 1350-4
 Borghi, Elena, 950-5
 Boti, Zsuzsa, 1012-17
 Bottomley, Frank, 1726-32
 Boubel, Jean Claude, 1506-10
 Boylan, Michael J., 1185-9
 Bradley, Geraldine, 522-6
 Bregeault, Jean Marie, 1411-17
 Brisdon, Brian J., 291-5
 Brown, Alan J., 1776-81
 Brown, Donald H., 199-201
 Brown, Lesley C., 877-9
 Brown, Michael P., 516-22, 1540-4
 Brown, Peter, 173-7
 Browning, Jane, 872-6
 Bruce, Donald M., 64-7, 1627-31
 Bruce, Michael I., 687-94
 Brunner, Henri, 1664-70
 Brunvoll, Jon, 299-302
 Bryan, Eric G., 196-8
 Bulcke, Petra, 861-8
 Bulloch, Gordon, 764-9
 Bullock, Joseph I., 36-9, 1536-40
 Burgess, John, 244-7, 996-1000, 1001-8, 1086-90, 1447-51, 1577-81
 Burt, Jennifer C., 1385-7, 1387-92
 Butler, Graham, 1654-8
 Calderazzo, Fausto, 1189-95
 Calhoun, Harry P., 1342-9
 Cali, Rosario, 1090-4
 Calligaris, Mario, 279-82
 Campbell, Michel J. M., 1090-4
 Canada, Larry G., 1573-6
 Canti, Giorgio, 1269-73
 Cardaci, Giuseppe, 695-8
 Cardin, Christine J., 46-50
 Cardin, David J., 46-50
 Cariati, Franco, 1018-24
 Carmona-Guzman, Ernesto, 1139-43
 Carroll, W. Eamon, 1472-8
 Carter, Forrest L., 1686-90
 Cattalini, Lucio, 12-14, 728-34
 Catton, Graham A., 181-4
 Cavell, Kingsley J., 1311-13
 Celon, Eloisa, 1618-21
 Cenini, Sergio, 1155-60
 Chagas, Aecio P., 1102-4
 Chapman, Carey A., 1807-13
 Chatt, Joseph, 165-9, 1638-47, 1654-8, 1766-76
 Chaudret, Bruno N., 1739-45
 Chini, Paolo, 459-63, 463-7
 Christou, George, 1423-5
 Ciani, Gianfranco, 463-7, 798-801
 Cinquantini, Arnaldo, 569-72, 569-72
 Ciriano, Miguel, 801-8
 Clark, R. J. H., 170-3
 Clark, Robin J. H., 1622-7, 1714-21
 Clay, Robert M., 577-83
 Clegg, William, 1452-4
 Clemente, Dore A., 373-80
 Cline, Susan J., 1051-7
 Coldbeck, Michael, 4-8
 Cole-Hamilton, David J., 454-9, 1739-45
 Collins, Michael P. S., 277-9
 Colquhoun, Howard M., 303-9, 944-7
 Connelly, Neil G., 50-3, 1375-9, 1532-6
 Cook, Alfred G., 173-7
 Cooksey, Brian G., 141-4
 Cooksey, Christopher J., 1814-20
 Cookson, Peter, 996-1000
 Cooper, Mervyn K., 587-92
 Corigliano, Francesco, 1329-33
 Cornock, Margaret C., 1195-200
 Corradi, Anna Bonamartini, 583-7
 Craddock, Stephen, 759-63
 Crease, Allan E., 1821-5
 Crichton, Oliver, 202-7, 208-15
 Crociani, Bruno, 1478-84
 Crocker, Christopher, 388-94
 Crook, Joseph R., 1152-4
 Csanyi, Laszlo J., 1012-17
 Cundy, Colin S., 427-33, 665-73
 Curic, Milisav, 566-9
 Curtis, Neil F., 68-76
 Cusumano, Matteo, 12-14, 1682-5
 Davies, Stephen G., 1510-14
 Davis, Kathryn M., 1098-102
 Day, J. Philip, 677-80
 Day, Peter, 1207-12
 Daykin, Helen, 1532-6
 Debuyst, Rene, 526-30
 De C. T. Carrondo, Maria A. A. F., 844-8
 Deeming, Antony J., 1201-6, 1490-6, 1497-501
 Degetto, Sandro, 12-14
 Dejeht, Fernand, 526-30
 Delpuech, Jean Jacques, 1506-10
 Demidowicz, Zenon, 50-3, 1532-6
 De Munno, Giovanni, 1549-54
 De Renzi, Augusto, 1392-7
 Desideri, Alessandro, 423-6
 Dessy, Giulia, 1549-54
 De Villardi, George C., 315-19
 De Waal, Dirk J. A., 340-7
 Dewan, John C., 968-72, 1528-32
 De Wet, J. Ferdinand, 592-7
 Diamantis, Alex A., 423-6
 Di Blasio, Benedetto, 1392-7
 Di Castro, Valeria, 950-5
 Dickinson, Roger J., 177-80
 Dieck, Ronald L., 173-7
 Dillon, Keith B., 1318-23, 1455-60, 1465-71
 Dilworth, Jonathan R., 1654-8
 Di Pasquale, Sebastiana, 1329-33
 Dodd, David, 1807-13, 1814-20
 Doppelberger, Johann, 1664-70
 Down, Michael G., 1407-11
 Downs, Anthony J., 809-17, 1755-61
 Drew, Michael G. B., 80-4, 511-16, 1098-102, 1176-9
 Duke, Brian J., 277-9
 Du Preez, Jan G. H., 592-7
 D'Urso, N. R., 170-3
 Eaborn, Colin, 357-68, 1288-94
 Eady, Colin R., 1358-63
 Earl, William L., 267-72
 Ebsworth, E. A. V., 272-6, 753-8, 759-63, 877-9, 1161-4, 1167-70
 Edward, Joyce M., 1161-4
 Edwards, Anthony J., 968-72, 1528-32, 1723-5
 Edwards, Dennis A., 1098-102
 Edwards, John, 295-8
 Egdel, Russell G., 1755-61
 Elson, Clive M., 165-9
 Empsall, H. David, 257-62, 1119-26
 Emsley, James W., 1355-8
 English, Robin B., 1379-85
 Ennis, Mary, 1185-9
 Erbe, Juergen, 1155-60
 Esperas, Steinar, 638-46
 Espley, David J. C., 57-61
 Eujen, Reint, 541-4
 Evans, Alwyn G., 57-61
 Evans, Dennis F., 315-19
 Evans, Jeffrey C., 57-61
 Evans, John, 18-25, 25-31, 626-34, 1355-8
 Evans, Sandra V., 160-5
 Fabbri, Luigi, 577-83
 Fachinetti, Giuseppe, 1398-403
 Fares, Vincenzo, 1549-54
 Favas, Mark C., 793-7
 Fawcett, J. Paul, 789-93
 Fendler, Janos H., 1226-32
 Ferguson, George, 253-6, 1131-4
 Fernandes, Terence R., 1024-31
 Ferrari, Rosa P., 1164-6
 Filby, Alan G., 1797-9
 Fillion, Gerard, 1686-90
 Fimminore, Stephen R., 1247-55
 Flaminio, Alberto, 454-9, 695-8
 Floriani, Carlo, 545-9, 1398-403
 Forsellini, Eleonora, 677-80, 818-21
 Forster, Alison, 196-8
 Forsyth, Michael I., 1363-74
 Fowles, Gerald A. W., 1658-61
 Gal, Ivan J., 549-52
 Galyer, Lee, 1403-7
 Gamsjaeger, Heinz, 496-500
 Gardiner, Derek J., 705-10
 Garner, C. David, 1311-13, 1350-4, 1582-9, 1848-54
 Garnier, Arlette, 53-6
 Garrick, Peter M., 416-18
 Gaudemer, Alain, 1807-13
 Gergely, Arthur, 964-8
 Gervasio, Giuliana, 222-7, 534-40
 Gibb, Terence C., 743-52
 Giesbrecht, Ernesto, 1610-17
 Giles, Harold F., Jr., 977-80, 1671-7
 Gill, Devinder S., 617-26
 Gill, J. Bernard, 1431-3
 Gillard, R. D., 152-8, 1444-7
 Giusto, Domenico, 798-801
 Glidewell, Christopher, 604-7
 Gmehling, Juergen, 960-4

- Goddard, Richard, 1247-55,
1255-60
Goel, Ram G., 253-6
Goetz, Jiri, 1134-8
Goggin, Peter L., 328-32,
388-94, 561-6, 872-6
Goodall, Brian L., 687-94
Goodall, David C., 1431-3
Goodfellow, John A., 1195-200
Goodfellow, Robin J., 328-32,
561-6, 872-6
Goodgame, David M. L., 880-4,
1705-9
Goodgame, Margaret, 1294-7
Gorham, John D., 141-4
Gosden, Cary, 972-6
Gould, Robert O., 76-9, 769-75,
1167-70
Gowenlock, Brian G., 657-64
Graziana, Mauro, 279-82
Graziani, Rodolfo, 818-21,
1618-21
Green, Anthony R., 759-63
Green, Jennifer C., 1403-7
Green, Malcolm L. H., 1510-14
Green, Michael, 158-9, 309-14,
801-8, 1067-80, 1472-8,
1839-47
Greenhough, Trevor J., 303-9,
944-7
Greenwood, Norman N., 40-3,
237-44, 1144-5, 1146-52
Griffith, William P., 1411-17,
1501-6, 1599-602
Grigg, Ronald, 333-9
Grinter, Roger, 608-11
Gruenewald, Bernd, 1221-5
Guarini, Giulio G. T., 1484-9
Guastini, Carlo, 956-9
Gupta, B. Dass, 1807-13,
1821-5
Haase, Wolfgang, 1594-8
Hadjiliadis, Nick, 1691-5
Haegele, Gerhard, 9-12
Hahn, James E., 1232-6
Haines, Raymond J., 1379-85
Haines, Robert I., 244-7,
1001-8, 1447-51
Haji, Ali H., 705-10
Haley, Martin J., 1407-11
Halfpenny, Michael T., 1662-3
Hall, Brian, 986-9
Hamill, Delphia, 433-40
Hamor, Thomas A., 647-50
Hancock, Robert D., 228-34,
1438-44
Hargittai, Istvan, 299-302,
861-8
Harman, Mary E., 181-4
Harris, Paul J., 403-12, 1009-12
Harris, Robin K., 9-12
Harrison, Neil C., 1337-42
Harrison, Philip G., 1274-8
Harrison, W. David, 1431-3
Hart, F. Alan, 181-4
Hartley, Frank R., 115-23,
123-31
Hartshorn, Angus J., 348-56
Hartsuiker, Janneke G., 1425-30
Haszeldine, Robert N., 1024-31
Hatfield, William E., 868-71,
1051-7
Hauge, Robert H., 433-40
Hawkes, Geoffrey E., 181-4
Hay, Robert W., 556-60,
1046-51, 1131-4
Haycock, Derek E., 1785-90,
1791-6
Head, Robert A., 885-9, 889-95
895-901, 901-9, 909-12,
913-15, 1638-47
Healy, Keith P., 972-6
Henner, Bernard J. L., 272-6
Herak, Rajna, 566-9
Hermanek, Stanislav, 944-7
Herron, Norman, 394-9, 1282-8
Heys, Peter N., 257-62, 1119-26
Hills, David J., 776-82, 782-8
Hitchcock, Peter B., 826-36
Hodgson, Derek J., 1051-7
Holbrook, Jack B., 1631-4
Hollis, Stephen, 511-16
Holloway, John H., 64-7,
1627-31
Horvath, Istvan, 1012-17
Hoskins, Bernard F., 320-8
Hough, Edward, 15-18
Howard, Joseph, 921-5
Howard, Judith A. K., 403-12,
412-16, 734-40, 801-8,
1472-8, 1839-47
Howarth, Oliver W., 503-6,
1776-81
Howden, Martin E., 1577-81
Howie, R. Alan, 1797-9
Howlader, Nepal C., 1350-4,
1582-9, 1848-54
Hsian-Yun, Wang, 638-46
Hubberstey, Peter, 1407-11
Huber, Friedo, 960-4
Hughes, Martin N., 530-4,
1634-7
Humphries, Adrian P., 1514-23,
1523-8
Hunt, James, 1240-6
Hunt, Martin M., 467-74, 474-9
480-2
Hunter, William E., 1189-95
Hurst, Nicholas W., 561-6,
872-6
Hursthouse, Michael B.,
1314-18, 1334-7, 1490-6
Hutton, Jennifer A., 1176-9
Hyde, Eileen M., 1696-705
Ige, Jide, 148-51
Inubushi, Toshiro, 1298-304
Irving, Roger J., 399-402
Isabirye, David A., 740-3
Jackson, Ronald A., 789-93
James, Bruce D., 710-22
Jameson, Geoffrey B., 185-91,
191-6
Jameson, Reginald F., 43-5
Jarrold, Martin, 503-6
Jeeves, Ian, 880-4
Jeffreys, John A. D., 144-7
Johns, Keith W., 1294-7
Johnson, Antony, 980-5
Johnson, Brian F. G., 196-8,
369-73, 381-7, 626-34, 673-6,
1358-63, 1554-68
Johnson, G. A., 1375-9
Johnson, Michael D., 1807-13,
1814-20, 1821-5
Johnston, James H., 68-76
Jones, Gordon R., 968-72,
1528-32
Jones, John G., 1709-14
Jones, Richard A., 446-53,
1063-6
Jorge, Renato A., 1102-4
Kane, Lorna, 141-4
Kano, Koji, 1226-32
Kariuki, David N., 262-7
Kasrai, Masoud, 1791-6
Katz, Nestor E., 1603-6
Keable, Jane, 986-9
Keasey, Alan, 1825-30, 1830-9
Keat, Rodney, 634-8, 764-9
Kemmitt, Raymond D. W.,
1577-81
Kemp, Terence J., 569-72
Kennedy, John D., 40-3, 237-44
1146-52
Kepert, David L., 133-7, 137-41
793-7, 1781-4
Kerridge, David H., 1589-93
Kessler, Katerina, 328-32
Kettle, Sidney F. A., 262-7
Keturah, Catherine, 1057-62
Khaled, F. Mahnaz, 1631-4
Khan, M. A., 915-18
Kiernan, Patrick M., 1127-30,
1411-17
Killops, Stephen D., 1247-55,
1255-60, 1260-9
Kimura, Eiichi, 104-10, 247-53,
1081-5
King, Trevor J., 333-9, 1350-4
Kiss, Tamas, 964-8
Kita, W. George, 467-74, 474-9
Kitano, Ryuichiro, 234-7
Knoche, Wilhelm, 1221-5
Knox, Selby A. R., 403-12,
1009-12, 1240-6, 1247-55,
1255-60, 1260-9, 1514-23,
1523-8
Kobayashi, Akiko, 482-5
Kodama, Mutsuo, 104-10,
247-53, 1081-5
Kolthammer, Brian W. S., 31-5
Kongkathip, Boonsong, 333-9
Koon, Seah Sen, 185-91
Kunze, Kenneth R., 433-40
Kurosawa, Hideo, 234-7
Kyle, James H., 133-7, 137-41,
1781-4
Labarre, Jean Francois, 861-8
Lagow, Richard J., 541-4
Laing, Michael, 1032-6
Lampe, Paul A., 1324-8
Landi, Alberto, 545-9
Lanfredi, Anna Maria Manotti,
552-6
Lappert, Michael F., 46-50,
348-56, 427-33, 665-73,
734-40, 826-36, 837-44
Lappin, A. Graham, 1606-9
Larkworthy, Leslie F., 1236-40
Lati, Joseph, 1105-18
Lau, Aldrich N. K., 1573-6
Leach, Grahame A., 1705-9
Legzdins, Peter, 31-5
Leigh, G. Jeffery, 1638-47,
1654-8
Lenarda, Maurizio, 279-82
Levason, William, 177-80,
1662-3
Lewis, Jack, 196-8, 369-73,
440-6, 626-34, 673-6,
1358-63
Liao, Sarah S. T., 1180-5
Lim, Meng Chay, 726-8
Lin, Ivan J. B., 1726-32
Lindsell, W. Edward, 657-64
Lloyd, D. Robert, 1403-7
Lockhart, Joyce C., 611-17
Lockman, Bill L., 1807-13,
1814-20
Louw, Wynand J., 340-7
Luchinat, Claudio, 1269-73
Ludi, Andreas, 1127-30
Ludwick, Adriane G., 1573-6
Ludwick, Larry M., 1573-6
Lukehart, Charles M., 93-5
Lusty, James R., 530-4
Lyle, Samuel J., 601-4
Mabbs, Frank E., 1350-4,
1582-9, 1848-54
McArdle, Patrick, 1678-82
McAuley, Alexander, 1606-9
McAuliffe, Charles A., 177-80,
1662-3
McCleverty, Jon A., 467-74,
474-9, 480-2
McDonald, Walter S., 40-3,
1119-26
McDougall, Gloria J., 1438-44
MacFie, John, 144-7
MacKay, Kenneth M., 506-11,
722-6, 1569-73, 1752-5
McKee, Vickie, 80-4, 522-6
Mackey, Denis J., 160-5, 702-4
McKinley, Gordon C., 199-201
McKinney, Ronald J., 403-12,
1009-12
McMeeking, Robert F., 160-5
McPartlin, Mary, 587-92, 673-6
McPhail, Andrew T., 1582-9,
1848-54
McQuillan, Geoffrey P., 1460-4
McVicker, Elizabeth M., 9-12
Magon, Luciano, 569-72
Maitlis, Peter M., 617-26,
849-57, 857-61, 1305-11,
1825-30, 1830-9
Mak, Pak-Wing, 216-21
Malatesta, Maria Carlotta,
1358-63
Malik, K. M. Abdul, 1314-18,
1334-7
Mallinson, Leslie G., 872-6
Manassero, Mario, 798-801
Mann, Brian E., 467-74, 1761-6
Manning, A. R., 1185-9
Marangoni, Giampaolo, 818-21,
1618-21
March, Frank C., 185-91
Marchetti, Fabio, 545-9,
1398-403
Marganian, Vahe M., 1167-70
Margrave, John L., 433-40
Marshalsea, John, 1098-102
Marsicano, Fabrizio, 228-34
Martin, John W. L., 68-76
Martin, Raymond L., 320-8,
702-4
Martinengo, Secondo, 459-63,
463-7
Martins, Joaniel M., 1610-17
Masson, Charles R., 1134-8,
1342-9
Masters, Christopher, 1213-20
Matheson, Trevor W., 196-8
Matheson, Trevor W., 626-34
Mavani, Ishwerlal P., 1189-95
May, Peter M., 1433-8
Mazzi, Ulderico, 373-80
Mehrotra, Raj Narain, 681-6
Mekhail, Fikry M., 996-1000,
1001-8
Mellini, Marcello, 1398-403
Mentasti, Edoardo, 61-3
Mertis, Konstantinos, 1403-7
Merz, Ludwig, 1594-8
Meseri, Yisay, 85-90
Meyerstein, Dan, 1105-18
Miller, Richard W., 1582-9
Milone, Luciano, 534-40
Mingos, D. Michael P., 1363-74
Mitchell, Terence N., 960-4
Mitsudo, Takeaki, 1298-304
Moeller, Therald, 173-7
Monacelli, Fabrizio, 950-5
Moore, Peter, 394-9, 1282-8

- 1324-8, 1776-81
Moorhouse, Stephen, 1821-5
Morazzoni, Franca, 1018-24
Morgan, Peter H., 57-61
Morishima, Isao, 1298-304
Morris, John H., 141-4
Mortimer, Jonathan, 57-61
Morton, Stephen, 1452-4
Moser, Wolf, 1797-9
Moss, Gerard P., 181-4
Muir, Kenneth W., 46-50
Murati, Ivo, 500-2
Murray, Martin, 872-6, 1337-42
Muscarella, Joseph C., 1152-4
Nachbaur, Edgar, 921-5
Nagel, Bertram, 861-8
Nakajima, Masayuki, 482-5
Nakanishi, Hiroshi, 1298-304
Nardelli, Mario, 131-3, 583-7
Nassimbeni, Luigi R., 1379-85
Natile, Giovanni, 728-34
Nelson, Jane, 522-6
Nelson, S. Martin, 80-4, 522-6
New, Lucy, 1490-6
Newell, J. Kay, 1189-95
Nicholls, Christopher J., 1785-90, 1791-6
Nicholson, David G., 15-18
Niciecki, Edmund, 1721-3
Nicolini, Marino, 1478-84
Nielson, Alastair J., 1501-6
Nikolic, Ruzica M., 549-52
Nimry, Tayseer, 1232-6
Nisbet, Martin P., 1455-60
Nixon, John F., 885-9, 889-95, 895-901, 901-9, 909-12, 913-15
Nnadi, Robert, 148-51
Nolte, Magriet J., 932-7, 1040-2, 1043-6
Noltes, Jan G., 1800-6
Nome, Faruk, 1226-32
Norton, Jack R., 626-34
Norton, Michael C., 1119-26
Nyathi, Jeffrey Z., 1067-80
O'Brien, P., 1444-7
Oddy, Peter R., 572-7
Odell, Kevin J., 357-68, 1288-94
Ogini, William O., 253-6
Ojo, Jonathan Folorunso, 148-51
Olabe, Jose A., 1603-6
Oliphant, Valerie, 1240-6
Olubuyide, Olusegun, 148-51
Omer, M. M., 918-20
Onan, Kay D., 1582-9, 1848-54
Orchard, Anthony F., 1755-61
Orchard, David, 1654-8
Owen, John D., 1418-23
Oxton, Ian A., 1460-4
Pahor, Nevenka Bresciani, 279-82
Palmer, Richard Alan, 977-80, 1671-7
Panunzi, Achille, 1392-7
Paoletti, Piero, 577-83
Paolucci, Gino, 818-21, 1618-21
Parish, R. V., 177-80
Parkes, Stephen, 1311-13
Parr, William J. E., 1776-81
Parrett, Frederick W., 1536-40
Pasquali, Marco, 545-9
Pavlovic, Dusanka, 500-2
Paxton, Keith, 647-50
Pearman, Alan J., 1766-76
Pedone, Carlo, 1392-7
Peguy, Alain, 1506-10
Pelizzetti, Ezio, 61-3
Pelizzi, Corrado, 131-3
Pelizzi, Giancarlo, 131-3
Peloso, Arnaldo, 699-702
Petkovic, Djordje M., 1-4
Pettit, Leslie D., 286-90
Pfeffer, Michel, 1472-8
Phillips, Ralph L., 1732-5, 1736-9
Phillips, Richard P., 403-12
Pickett, Christopher J., 1638-47
Pico, Carlos, 948-50
Pidcock, Alan, 357-68, 1288-94
Pilcher, Geoffrey, 1311-13
Pinkerton, A. Alan, 85-90, 267-72, 989-96
Piplani, Dharam P., 556-60, 1046-51, 1131-4
Pitteri, Bruno, 728-34
Pizzotti, Maddalena, 1155-60
Plesek, Jaromir, 944-7
Pletcher, Derek, 972-6
Pneumatikakis, George, 1691-5
Poe, Anthony, 789-93
Pombeiro, Armando J. L., 165-9
Poon, Chung-Kwong, 216-21, 740-3, 1180-5
Pope, Lynn, 1032-6
Porta, Francesca, 1155-60
Porta, Piero, 956-9
Post, Michael L., 1536-40
Pramauero, Edmondo, 61-3
Prelesnik, Bogdan, 566-9
Prescott, Aileen M., 328-32
Proud, Jill, 801-8
Puddephatt, Richard J., 516-22, 980-5, 1540-4, 1732-5, 1736-9
Pulham, Richard J., 1407-11
Pye, Peter L., 826-36, 837-44
Raithby, Paul R., 673-6
Randaccio, Lucio, 279-82
Rankin, David W. H., 753-8
Rashidi, Mehdi, 516-22, 1540-4
Raynor, J. Barrie, 423-6
Reed, F. J. S., 877-9
Reed, Francis J. S., 272-6, 1161-4, 1167-7
Reedijk, Jan, 1170-5
Reeve, Roger N., 1318-23, 1465-71
Reimann, Rolf H., 932-7, 1036-9, 1043-6
Reisner, M. George, 1664-70
Rest, Antony J., 202-7, 208-15, 651-6
Restivo, Roderic J., 253-6, 1131-4
Ribeiro da Silva, Manuel A. V., 399-402
Rice, David A., 1658-61
Ricevuto, Vittorio, 1682-5
Richards, Raymond L., 165-9, 1478-84, 1766-76
Ridge, Brian, 1423-5
Rieder, Charly, 85-90
Rios-Gutierrez, E., 948-50
Rizzarelli, Enrico, 1090-4
Roberts, David L., 996-1000, 1086-90
Roberts, Paul J., 253-6
Robertson, Donald R., 486-95
Robertson, Glen B., 587-92
Robertson, Heather E., 753-8
Robinet, Germaine, 861-8
Robinson, Ward T., 185-91, 191-6
Robinson, William R., 1232-6
Robson, Anita C., 611-17
Rodley, Gordon A., 191-6
Rogers, David E., 115-23, 123-31
Rosini, Carlo, 822-6
Rossetti, Rosanna, 222-7, 534-40
Rossi, Roberto, 569-72
Rothwell, Ian P., 1490-6, 1497-501
Royston, Geoffrey H. D., 165-9
Rozsondai, Bela, 861-8
Russell, David R., 64-7, 1627-31
Russell, Michael J. H., 849-57, 857-61
Rycroft, David S., 764-9
Rydon, H. N., 1423-5
Saito, Taro, 482-5
Salama, S. B., 915-18, 918-20
Sales, Keith D., 1314-18
Salmon, Dennis J., 1232-6
Salvadori, Piero, 822-6
Sammartano, Silvio, 1090-4
Sansoni, Mirella, 459-63, 463-7, 798-801
Sappa, Enrico, 419-23, 552-6
Sasaki, Torahiko, 234-7
Sasaki, Yukiyo, 482-5
Savory, Christopher G., 237-44
Scaramuzza, Lucio, 1549-54
Schmid, Guenter, 1385-7, 1387-92
Schmulbach, C. David, 173-7
Schmutzler, Reinhardt, 1662-3
Scholes, Gary, 309-14
Schroeder, Martin, 1599-602
Schwarzenbach, Dieter, 989-96
Scott, Caron, 1067-80
Seccafava, Andrea, 1269-73
Seddon, Kenneth R., 516-22, 1540-4
Seip, Ragnhild, 299-302
Semprini, Elvio, 695-8
Septe, Bernard, 1807-13
Shakir, Riz, 844-8
Shanton, Kenneth J., 1658-61
Shaw, Bernard L., 257-62, 1119-26, 1696-705
Sheldrick, George M., 673-6
Shepherd, Ian, 1696-705
Sherlock, Hal, 1678-82
Shibahara, Takashi, 95-9, 100-4
Shrimanker, Kishore, 1634-7
Shurvell, Herbert F., 710-22
Sieber, Werner, 598-601
Sime, Wilma J., 76-9, 1647-53
Singh, Balbir, 657-64
Singleton, Eric, 340-7, 926-31, 1032-6, 1036-9, 1040-2, 1043-6
Singleton, Joy E., 340-7
Skapski, Andrzej C., 844-8
Slyudkin, O. P., 152-8
Smith, Barry C., 1631-4
Smith, Brian E., 710-22
Smith, W. Ewen, 199-201
Snaith, Ronald, 986-9
Sodeau, John R., 651-6
Sovago, Imre, 964-8
Sowerby, D. Bryan, 1094-8, 1544-8
Spek, Anthony L., 1800-6
Spencer, John L., 801-8, 1337-42, 1839-47
Spinicci, Roberto, 1484-9
Sridhara, Narendra S., 1577-81
Stanghellini, Pier Luigi, 222-7, 534-40
Staves, John, 237-44, 1144-5, 1146-52
Stefani, Ferdinanda, 695-8
Stephenson, G. Richard, 369-73
Stephenson, T. Anthony, 761-9, 486-95, 769-75, 1195-200, 1647-53
Stobart, Stephen R., 938-43
Stone, F. Gordon A., 309-14, 403-12, 687-94, 801-8, 1009-12, 1067-80, 1337-42, 1472-8, 1839-47
Straughan, Brian, 705-10
Strumolo, Donatella, 459-63
Sustra, Ante, 500-2
Swanwick, Michael G., 158-9
Swash, John L. M., 286-90
Sykes, A. Geoffrey, 95-9, 100-4
Szil, Zsuzsa, 1012-17
Tajmir-Riahi, Heidar-Ali, 36-9
Takegami, Yoshinobu, 1298-304
Tani, Maria E. Vidoni, 583-7
Tasker, Peter A., 1057-62
Taylor, David J., 651-6
Taylor, Donald, 320-8
Taylor, Nicholas J., 1536-40
Tempest, Andrew C., 295-8
Ten Hoedt, Richard W. M., 1800-6
Thomas, Patrick D. P., 809-17, 1755-61
Thompson, David G., 634-8
Thompson, Maurice E., 611-17
Thompson, Stephen J., 1305-11
Thomson, Andrew J., 608-11
Thomson, Mary A., 769-75
Thornback, John R., 110-15
Thornton, Edward W., 1274-8
Thunder, Anne E., 1407-11
Tipping, Anthony E., 1024-31
Tiripicchio, Antonio, 419-23, 552-6
Tiripicchio Camellini, Marisa, 419-23
Toma, Henrique E., 1610-17
Tomlinson, Anthony A. G., 950-5, 956-9, 1549-54
Torrence, G. Paull, 93-5
Tosi, Lucia, 53-6
Traverso, Orazio, 569-72
Trigwell, Keith R., 237-44
Trombe, Jean Christian, 1746-52
Trotter, Jill, 1057-62
Tspis, Constantinos A., 801-8
Turner, Keith, 348-56
Turtle, Philip C., 1622-7, 1714-21
Twigg, Martyn V., 1709-14
Tyson, Philip D., 611-17
Urch, David S., 1785-90, 1791-6
Vaglio, Gian A., 1164-6
Valle, Mario, 1164-6
Van der Stok, Erwin, 340-7, 926-31
Van der Woude, Constance, 1213-20
Van Doorn, Johannes A., 1213-20
Van Koten, Gerard, 1800-6
Van Ooijen, Johannes A. C., 1170-5
Vasic, Parle, 566-9
Veiga, M. L., 948-50
Verma, Rajendar D., 1544-8
Vichi, Eduardo J. S., 369-73
Villa, Angela Chiesi, 956-9
Vitagliano, Aldo, 1392-7
Vitali, Dario, 1189-95
Von Felton, Hans, 496-500

- Vosper, Alan J., 1721-3
Waddington, Thomas C., 921-5,
1318-23, 1455-60, 1465-71
Wade, Kenneth, 986-9
Wagner, Anton J., 1425-30
Wainwright, Kevin P., 440-6
Wakatsuki, Yasuo, 1278-82
Wallace, Ian H. M., 611-17
Wallbridge, Malcolm G. H.,
303-9, 572-7, 944-7
Wallis, Helen L., 530-4
Walsh, Peter T., 601-4
Walter, Robert H., 381-7
Walton, Richard A., 1232-6
Wasif, Saad, 915-18, 918-20
Wasson, John R., 1051-7
Watanabe, Yoshihisa, 1298-304
Webber, M. J., 1785-90
Welch, Alan J., 1067-80,
1363-74
Wellings, Paul, 996-1000
Wernli, Beat, 496-500
Whitcomb, David R., 1671-7
White, Colin, 617-26, 849-57,
857-61, 1305-11
White, Peter S., 1726-32
Whitelock, John D., 1161-4
Wiech, Gerhardt, 1785-90
Wilkinson, Geoffrey, 110-15,
446-53, 454-9, 1063-6,
1139-43, 1403-7, 1739-45
Williams, David R., 1433-8
Wimbledon, Peter E., 1634-7
Wolfers, Pierre, 1686-90
Wong, Fook Sin, 1752-5
Wong, Kenneth, 673-6
Woodward, Peter, 403-12,
412-16, 1067-80, 1247-55,
1255-60
Woolf, Alfred A., 291-5
Yamase, Toshihiro, 283-5
Yamazaki, Hiroshi, 1278-82
Yates, Alan, 849-57, 857-61
Yavari, Ahmad, 1236-40
Yin, Candido Choo, 1201-6
Young, Ian M., 1528-32
Yuen, Choi-Kwan, 427-33
Zandomeneghi, Maurizio, 822-6
Zocchi, Marcello, 1018-24
Zsigrai, Istvan J., 549-52

SUBJECT INDEX, 1978

ACETAMIDINE

Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetylamidine complexes of rhodium and iridium, 50-3

ACETATE

Structural studies of steric effects in phosphine complexes. Part 3. The synthesis, characterization and molecular structure of diacetato(tris(tert-butyl)phosphine)mercury(II), 253-6
Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9
Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyltetrahydrotetraosmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-tetrakis(tricarbonyl)osmium($4Os-Os$), 673-6
Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
Neutral, acetate-bridged, binuclear alkyls of ruthenium(III), 1063-6
Metal complexes of sulphur ligands. Part 17. Reaction of palladium(II) and platinum(II) monothiobenzoates with various Lewis bases and further studies on complexes containing related ligands, 1195-200
Crystal structure of tetrakis- μ -trifluoroacetato-bis(triaqua(trifluoroacetato)praseodymium(III)), 1544-8

ACETYLIDE

Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodiimide (cyanamide) 1407-11

ACID

Complexes of D-, L-, DL-, and meso-tartaric acid with hydrogen and oxovanadium(IV) cations, 286-90

ACTINIDE

The chemistry of uranium. Part 20. Tetraphenylphosphonium pentachloro-oxouranate(IV): crystal structure and bonding characteristics, 592-7

ACYL

Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14

ADDN

Preparation of (η -cycloocta-1,5-diene) halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7

Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), ruthenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridoruthenium(III), 348-56

ALDRIN

Crystal structure of exo-6-chloromercurio-6,7-dihydro-exo-7-methoxyaldrin (1,2,3,4,10,10-hexachloro-exo-6-chloromercurio-1,4,4a,5,6,7,8,8a-octahydro-endo,exo-1,4:5,8-dimethano-exo-7-methoxynaphthalene), 1573-6

ALK EARTH

The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64
Soft-sphere ionic radii for Group 1 and Group 2 metal halides and ammonium halides, 1631-4

ALKALI

Crystal structures of octaccesium and octarubidium docosaniobates 968-72

ALKALI METAL

Co-condensation reactions of uranium tetrafluoride and

hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40

Ligands for the alkali metals. Part 4. Nuclear magnetic resonance of crown ethers with alkali-metal ions, 611-17

Reactions of tellurium oxides with alkali-metal oxides and hydroxides, 948-50

Spectroscopy and reactions of copper(II), nickel(II), and cobalt(III) compounds in molten nitrates, 1589-93

Soft-sphere ionic radii for Group 1 and Group 2 metal halides and ammonium halides, 1631-4

A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4

ALKANE

Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5

ALKENE

Hydrogen-1 nuclear magnetic resonance evidence for trans addition in oxythallation of acyclic olefins, 234-7

Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14

Rhodium(I) complexes of diallyl ethers and related compounds, 333-9

Preparation of (η -cycloocta-1,5-diene) halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7

Preparation and reactions of triphenylphosphine and triphenyl phosphite complexes of (benzylideneacetone)dicarbonyliron(0), 369-73

The chemistry of carbonyl(phenylethynyl)bis(triphenylphosphine)iridium(I), 381-7

The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26

He(I) photoelectron spectra of tetracarbonyliron complexes of Group 5 ligands and of olefinic ligands, 695-8

Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15

Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine) ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6

Synthesis and dynamic behaviour of bis(ethylene)(tertiary phosphine)platinum complexes, 1337-42

The structure of ac-dichloro-b-ethylene-d-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8

Addition reactions on coordinated olefinic ligands. Part 8.

Platinum(II) complexes of 1,1-dimethylallene and their reaction with amines. Molecular structure of the zwitterionic derivative dichloro(1-(NN-diethylammoniomethyl)-2-methylprop-1-enyl)(triphenylphosphine)platinum(II), 1392-7

Reactions of dodecacarbonyl-triangulo-triruthenium and dodecacarbonyltetrahydrotetraruthenium with mixtures of cyclic polyolefins, 1523-8

Reaction of tricarbonyl(2- η -hexadienyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82

Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45

Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20

Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)

(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47

ALKENYL

An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonylbis(η -dienyl)isocyanidediiron complexes, 1185-9

Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5

ALKYL

Electron spin resonance studies of Ziegler-type catalysts. Part 2. Identification and spectra of some dialkylidene(η -cyclopentadienyl)vanadium(IV) complexes, 57-61

Vibrational spectra of some trichloromethyl- and trifluoromethylmercury(II) compounds, 328-32

Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68

Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53

Reactions of bis(trifluoromethyl)mercury: the synthesis and properties of methyl(trifluoromethyl)-stannanes and -plumbanes, 541-4

Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6

The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64

Solvation of mercury(II) halides and alkylmercury(II) halides by liquid ammonia: a Raman spectroscopic study, 705-10

Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40

Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5

Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12

Neutral, acetate-bridged, binuclear alkyls of rhenium(III), 1063-6

Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80

Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43

Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52

Crystal and molecular structure of di- μ -trimethylsilylmethyl-bis((trimethylphosphine)(trimethylsilylmethyl)chromium(II)) (4Cr-Cr), 1314-18

Crystal structures of methyl(L-tyrosinato)mercury(II) monohydrate and (L-(2-amino-4-phenylbutanoato))methylmercury(II), 1324-8

Crystal and molecular structure of tri- μ -chloro-hexakis(trimethylsilylmethyl)-triangulo-trirhenium(III), 1334-7

Photoelectron spectra of some transition metal alkyls and oxoalkyls, 1403-7

1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84

Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47

ALKYNE

Synthesis and molecular structure of bis(μ_4 -but-1-yne)-undecacarbonyl-quadrato-tetrairon (4 Fe-Fe), 419-23

The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2

Synthesis and crystal structure of heptacarbonyl- μ_5 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangulo-triiron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a metal-atom cluster, 552-6

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26

Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34

Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63

Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5

Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80

Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarboxylferrates and tricarboxyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304

Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403

Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81

Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602

ALKYNYL

Unsaturated σ -hydrocarbyl transition-metal complexes. Part 4. Crystal and molecular structure of trans-chlorobis(diethylphenylphosphine)(phenylethynyl)platinum(II) and comments on the relative trans influence of various carbon ligands, 46-50

The chemistry of carbonyl(phenylethynyl)bis(triphenylphosphine)iridium(I), 381-7

Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81

Group 1B organometallic chemistry. Part 25. Crystal and molecular structure of 1,2,3,1,4,5,2,3,6,4,5,6-tetrakis- μ_3 -2-dimethylaminophenyl-2,5,3,4-bis- μ_2 -4-tolylethynyl-octahydro-hexacopper(II), 1800-6

ALUMINIUM

Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5

Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14

Preparation of uncoordinated hydridoaluminium tetrahydroborate compounds, $\text{Al}(\text{BH}_4)_3\text{-H}_x$ ($x = 1$ or 2), and alane (AlH_3) species, 572-7

Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601

Single-crystal Raman and infrared study of aluminium trichloride hexahydrate, 782-8

Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulfoxide-sulphur dioxide, 1431-3

Photoelectron spectra of metal tetrahydroborates, 1755-61

Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulfoxide)aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81

The electronic structure of magnesium dialuminium tetraoxide (spinel) using X-ray emission and X-ray photoelectron spectroscopies, 1785-90

AMIDE

Some oxygen-donor complexes of cyclopentadienyluranium(IV)

- halides, 295-8
- Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
- AMINO ACID**
- Assignment of the proton-association constants for 3-(3,4-dihydroxyphenyl)alanine (L-dopa), 43-5
- Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino acids, 152-8
- Gold complexes of L-cysteine and D-penicillamine, 199-201
- Single-crystal electron spin resonance and electronic spectra of bis(β -alaninato)copper(II) hexahydrate, 526-30
- Mixed-ligand complexes of palladium(II). Part 3. Diaqua(ethylenediamine)palladium(II) complexes of L-amino acids, 726-8
- Effect of mixed-ligand complex formation on the ionization of the pyrrole hydrogens of histamine and histidine, 964-8
- Base hydrolysis of amino-acid esters and amides in the coordination sphere of cobalt(III). Part 3. Hydrolysis of methyl and ethyl 4-aminobutanoate, 1046-51
- Crystal structures of methyl(L-tyrosinato)mercury(II) monohydrate and (L-(2-amino-4-phenylbutanoato))methylmercury(II), 1324-8
- Computer simulation of metal-ion equilibria in biofluids. Part 2. Formation constants for zinc(II)-citrate-cysteinate binary and ternary complexes and improved models of low-molecular-weight zinc species in blood plasma, 1433-8
- The isomers of α -amino-acids with copper(II). Part 4. Catalysis of the racemization of optically active alanine by copper(II) and pyruvate in alkaline solution, 1444-7
- Kinetics of reaction of imidazole, glycine, and L-histidine with the aquapentacyanoferrate(II) ion, 1610-17
- ANTIMONY**
- Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80
- AQUATION**
- A damped nonlinear least-squares computer program (DALSFRK) for the evaluation of reaction rate constants, 123-31
- Reactions of platinum(II) complexes. Part 2. Catalysis of the aquation of tetrachloroplatinate(II) ion by trichloro(η -ethylene)platinate(II) (Zeise's anion), 158-9
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- Carbonylhalogeno(o-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate o-phenylenebis(dimethylarsine), 1726-32
- ARENE**
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Cyclometallation reactions. Part 17. Comparative studies of the manganation and palladation of some substituted azobenzenes, 687-94
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- ARGON**
- Photochemistry of carbonyltrinitsylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
- Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
- Co-condensation reactions of uranium tetrafluoride and hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- AROYL**
- Use of aryltin compounds in the preparation of diaryl- and diaroyle-di- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- ARSINE**
- Infrared and Raman spectroscopic studies of conformations in liquid and solid triethyl-, diethyl(methyl)- and ethyldimethylamines, -phosphines, and -arsines, 388-94
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenedihydridoruthenium with a series of neutral donor ligands, 1036-9
- Preparation and structures of ruthenium(III) complexes containing tertiary arsines, tertiary phosphines, and isocyanides, 1152-4
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
- Reaction of tricarbonyl(2- η -hexadecienyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82
- Carbonylhalogeno(o-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate o-phenylenebis(dimethylarsine), 1726-32
- ARYL**
- Coordinative tin-oxygen interactions in dinitratodiphenyl(triphenylphosphine oxide)tin(IV), 131-3
- Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
- Use of aryltin compounds in the preparation of diaryl- and diaroyle-di- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered aniono(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
- Group 1B organometallic chemistry. Part 25. Crystal and molecular structure of 1,2,3,1',4,5',2',3',6',4',5',6'-tetrakis- μ_2 -dimethylaminophenyl-2,5',3,4-bis- μ_2 -4-tolylethynyl-octahedro-hexacopper(I), 1800-6
- Trans-influence of anionic, neutral, and bridging ligands on the nuclear magnetic resonance spectra of methyl- and fluorobenzyl-bis(dimethylglyoximate)rhodium(III) complexes. Some observations on bridge formation, 1807-13
- ARYLATION**
- Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
- ASCORBIC ACID**
- Kinetics and mechanism of oxidation of ascorbic acid by manganese(III) in aqueous acidic perchlorate media, 61-3
- AZAHEPTANEDIAMINE**
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- BARIUM**
- Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601
- The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64
- BERYLLIUM**
- A kinetic study of the formation of some unchelated and chelated beryllium(II) complexes in aqueous solutions, 1221-5
- BIGUANIDE**
- Structural studies on biguanide and related species. Correlation of protonation energy with molecular structure, 989-96
- BISMUTH**
- X-ray crystal structures of μ_4 -chloro-(tris(trichloro(thiosemicarbazonide)bismuth(III)))

- (tris(thiosemicarbazide)bismuth(III)) hexachlorobismuthate(III) chloride and catena- μ -chloro-dichlorobis(ethylenethiourea) bismuth(III), 583-7
- BLOOD PLASMA**
Computer simulation of metal-ion equilibria in biofluids. Part 2. Formation constants for zinc(II)-citrate-cysteinate binary and ternary complexes and improved models of low-molecular-weight zinc species in blood plasma, 1433-8
- BORANE**
A molecular-orbital evaluation of skeletal electron-counting procedures, 18-25
Effects of extra hydrogens on the electronic structures of five- and six-vertexed polyhedral boranes, 25-31
Dicarbonyl(η -cyclopentadienyl)iron(II) derivatives of pentaborane(9), 237-44
Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5
Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52
- BORAPHOSPHANE**
Preparation and structure of 1,4-dichloro-1,1,3,3-tetraphenylcatena-di(boraphosphane), $\text{BH}_2\text{Cl.PPh}_2\text{.BH}_2\text{.PPh}_2\text{Cl}$, 40-3
- BORON**
A molecular-orbital evaluation of skeletal electron-counting procedures, 18-25
Effects of extra hydrogens on the electronic structures of five- and six-vertexed polyhedral boranes, 25-31
Preparation and structure of 1,4-dichloro-1,1,3,3-tetraphenylcatena-di(boraphosphane), $\text{BH}_2\text{Cl.PPh}_2\text{.BH}_2\text{.PPh}_2\text{Cl}$, 40-3
Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
Dicarbonyl(η -cyclopentadienyl)iron(II) derivatives of pentaborane(9), 237-44
Carborane derivatives of the late- and post-transition elements. Part 1. Preparation and X-ray crystal structure of 3-diethylthiocarbamate-1,2-dicarba-3-aurododecaborane(11), 303-9
Crystal and molecular structure of hydrido(tetrahydroborato) bis(tricyclohexylphosphine)nickel(II), 482-5
Preparation of uncoordinated hydridoaluminium tetrahydroborate compounds, $\text{Al}(\text{BH}_4)_3 \cdot x\text{H}_2$ ($x = 1$ or 2), and alane (AlH_3) species, 572-7
Molecular vibrations of zirconium(IV) tetrahydroborate, a compound containing triple hydrogen bridges, 710-22
Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborate(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(11), 944-7
A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- BRUCITE**
The electronic structure of magnesium hydroxide (brucite) using X-ray emission, X-ray photoelectron, and Auger spectroscopy, 1791-6
- BUTADIENE**
Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14
- CADMIUM**
The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms, 228-34
Thermodynamics of metal complex formation in aqueous melts of calcium dinitrate-ammonium nitrate. Part 2. Cadmium(II) bromides, 549-52
Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- CAESIUM**
Crystal structures of octacaesium and octarubidium docosaniobates, 968-72
- CALCIUM**
A structural theory for nonstoichiometry. Part 4. Defect fluorite-type structures: vacancy superstructures in ordered calcium oxide-hafnium dioxide ternary oxides, 320-8
The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64
Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- CARBENE**
Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56
Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44
- CARBIDE**
New carbide clusters in the cobalt sub-group. Part 4. Synthesis and crystallographic characterization of μ -carbonyl-deca- μ -carbonyl-dicarbido-tetradecacarbonyl-polyhydro-dodecacarbonyl, 459-63
New carbide clusters in the cobalt sub-group. Part 5. Crystallographic characterization of deca- μ -carbonyl-carbido-octacarbonyl-polyhydro-octacarbonyl(2-) in its bis(benzyltrimethylammonium) salt, 463-7
- CARBODIIMIDE**
Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodiimide (cyanamide), 1407-11
- CARBONIC ANHYDRASE**
Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, 1269-73
- CARBONYL**
Evidence for the formation of the triaquatetracarbonylmanganese(I) cation and related derivatives from pentacarbonylchloromanganese, 4-8
Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium), 31-5
Cationic diaryltriazene, hydrido(diaryltriazene)-, and diarylacetonide complexes of rhodium and iridium, 50-3
Crystal structure of abede-pentacarbonyl- μ -fluoro-ghijk-pentafluororhenium(I)rhenium(V), 64-7
Ruthenium complexes containing Group 5B donor ligands. Part 5. Synthesis and crystal and molecular structure of acetone(carbonyl)chloro(trichlorostannio) bis(triphenylphosphine)ruthenium(II)-acetone (1/1), 76-9
Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5
Schiff-base complexes of ruthenium(II), 110-15
Carbon-13 nuclear magnetic resonance study of osmium complexes of the type $\text{Os}_2(\text{CO})_{10}(\text{H}X)$, 196-8
Photochemistry of carbonyltrinitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobalturon, 222-7
Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
Structure of (η -allyl)dicarbonyl(pentane-2,4-dionato)

- pyridinemolybdenum(II) in the solid and solution states, 291-5
- Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56
- Preparation and reactions of triphenylphosphine and triphenyl phosphite complexes of (benzylideneacetone)dicarbonyliron(0), 369-73
- Carbonyltrichlorotris(dimethylphenylphosphine)technetium-ethanol (1/1), the first seven-coordinate complex of technetium; position of this molecule in the C_3 family, 373-80
- The chemistry of carbonyl(phenylethynyl)bis(triphenylphosphine)iridium(I), 381-7
- Hydrocarbon complexes of iron, ruthenium, and osmium. 11.
- Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3,6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
- Crystal and molecular structure of μ -pentalenebis(dicarbonyl(trimethylgermyl)ruthenium), 412-16
- Synthesis and molecular structure of bis(μ -but-1-ynyl)-undecacarbonyl-quattro-tetrairon (4 Fe-Fe), 419-23
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- New carbide clusters in the cobalt sub-group. Part 4. Synthesis and crystallographic characterization of μ_3 -carbonyl-deca- μ -carbonyl-dicarbido-tetradecacarbonyl-polyhedro-dodecarrhodium, 459-63
- New carbide clusters in the cobalt sub-group. Part 5. Crystallographic characterization of deca- μ -carbonyl-carbido-octacarbonyl-polyhedro-octacobaltate(2-) in its bis(benzyltrimethylammonium) salt, 463-7
- Transition-metal carbonyl derivatives of the germanes. Part 6. The methylgermyl iron carbonyl system, 506-11
- Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
- Synthesis and crystal structure of heptacarbonyl- μ_3 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangulo-triiron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a metal-atom cluster, 552-6
- Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-5)tungstate(0), 587-92
- The magnetic circular-dichroism spectrum of matrix-isolated vanadium hexacarbonyl, 608-11
- Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylmethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyltetrahydrotetraosmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-tetrakis(tricarbonylosmium)(4Os-Os), 673-6
- He(I) photoelectron spectra of tetracarbonyliron complexes of Group 5 ligands and of olefinic ligands, 695-8
- Transition-metal carbonyl derivatives of the germanes. Part 7. Properties of complexes containing dimethylgermyliron carbonyl groups and their interconversion, 722-6
- Reaction mechanisms of metal-metal-bonded carbonyls. Part 19. Homolytic fission of bis(tetracarbonyl(triphenylphosphine)manganese)(Mn-Mn) as a path for thermal substitution, 789-93
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Fluorophosphine complexes of ruthenium and osmium. Part 4. Homobinuclear trichloro-bridged complexes of ruthenium(II), 901-9
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-*o*-tolyl phosphite iridium(III) complexes, 926-31
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80
- Some mononuclear seven-coordinate rhenium(III) carbonyl complexes; the crystal and molecular structure of (2,2-bipyridyl)tribromodicarbonylrhenium(III), 1098-102
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxy-OP)(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)- $\text{C}^1\text{PO}_2^-(\text{methyl isocyanide})\text{iridium(III)}$, 1119-26
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonylbis(η -dienyl)isocyanidediiron complexes, 1185-9
- Crystal and molecular structure of di- μ -bromo- μ -tetraphenyldiphosphane-bis(tricarbonyl)rhenium(II), 1189-95
- Triosmium clusters derived from benzylamine and benzyl alcohol: formation of a μ_3 -*o*-phenylene complex in the conversion of benzyl alcohol into benzene, 1201-6
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Organosulphur-transition metal chemistry. Part 4. The isomerism of μ -thio- and μ -seleno-bis(carbonyl(η -cyclopentadienyl)ruthenium) complexes, 1260-9
- Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarbonylferrates and tricarbonyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304
- The chemistry of polynuclear compounds. Part 31. Synthesis of undecacarbonylhydriotriosmate(1-) and its reaction with octadecacarbonylhexaossmium to give a carboxylate-bridged anionic enneaoxmium species, 1358-63
- Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di- μ -aryltio-bis(η -cyclopentadienyl)rhodium, 1375-9
- Reactions of metal carbonyl derivatives. Part 22. The crystal and molecular structures of dicarbonyl(η -cyclopentadienyl)(ethylthio)iron and μ -ethylthio-bis(dicarbonyl(η -cyclopentadienyl)iron) tetrafluoroborate, and a comparison of their molecular parameters, 1379-85
- Heteronuclear cluster systems. Part 12. Synthesis of μ -phenylphosphinediyl-bis(tetracarbonylcobalt) and 1,1,1,2,2,2,3,3,3-nonacarbonyl- μ_3 -phenylphosphinediyl-triangulo-dicobaltiron 1385-7
- Heteronuclear cluster systems. Part 13. Synthesis of μ -diphenylphosphido-bridged carbonylmetal complexes, and

- crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3-hexacarbonyl-1,3; 2,3-bis- μ -diphenylphosphido-triangulo-tricobalt, 1387-92
- Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14
- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- Reactions of dodecacarbonyl-triangulo-triruthenium and dodecacarbonyltetrahydrotetraruthenium with mixtures of cyclic polyolefins, 1523-8
- Binuclear diaryltriazenido- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- Synthesis and structure of some binuclear carbonyl complexes of platinum(II), 1540-4
- Structures of binary carbonyls and related compounds. Part 1. A new approach to fluxional behaviour, 1554-68
- Transition-metal carbonyl derivatives of the germanes. Part 9. Reactions of tetracarbonyldi(methylgermyl)iron with some covalent halides, 1569-73
- Rhenium carbonyl fluorides: preparation, crystal structure, and some properties of hexacarbonylrhenium(I) μ -fluoro-bis(pentafluororhenate(V)), 1627-31
- Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (-)-578-carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino)diphenylphosphine)nitrosylmolybdenum, 1664-70
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- Carbonylhalogeno(o-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate o-phenylenebis(dimethylarsine), 1726-32
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5
- Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5
- ### CARBORANE
- Carbaborane derivatives of the late- and post-transition elements. Part 1. Preparation and X-ray crystal structure of 3-diethylthiocarbamato-1,2-dicarba-3-auradodecaborane(II), 303-9
- Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborate(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(II), 944-7
- Molecular and crystal structure of 3,3-bis(triethylphosphine)-1,2-dicarba-3-platinadodecaborane(II), and molecular orbital analysis of the slip distortion in carbametalaboranes, 1363-74
- ### CARBOXYLATE
- Thermodynamic and spectroscopic properties of mixed complexes in aqueous solution. Copper(II) complexes of 2,2'-bipyridyl and dicarboxylic acids, 1090-4
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Crystal structures of methyl(L-tyrosinato)mercury(II) monohydrate and (L-(2-amino-4-phenylbutanoato))methylmercury(II), 1324-8
- The chemistry of polynuclear compounds. Part 31. Synthesis of undecacarbonylhydrotriosmate(1-) and its reaction with octadecacarbonylhexaosmium to give a carboxylate-bridged anionic enneaosmium species, 1358-63
- ### CATALYSIS
- Reactions of platinum(II) complexes. Part 2. Catalysis of the aqution of tetrachloroplatinate(II) ion by trichloro(η -ethylene)platinate(II) (Zeise's anion), 158-9
- Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64
- Reactions of strained organosilicon heterocycles with nonacarbonyliron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Tetramethylthiophene complexes of rhodium, iridium, palladium, and ruthenium, 857-61
- Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15
- Triosmium clusters derived from benzylamine and benzyl alcohol: formation of a μ_3 -o-phenylene complex in the conversion of benzyl alcohol into benzene, 1201-6
- Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403
- The isomers of α -amino-acids with copper(II). Part 4. Catalysis of the racemization of optically active alanine by copper(II) and pyruvate in alkaline solution, 1444-7
- ### CATECHOL
- Complexes of osmium(VI) with catechol and substituted catechols, 1501-6
- ### CHELATION
- A kinetic study of the formation of some unchelated and chelated beryllium(II) complexes in aqueous solutions, 1221-5
- ### CHROMATOGRAPHY
- Trimethylsilyl derivatives for the study of silicate structures. Part 5. Trimethylsilylation of diopase, 1342-9
- ### CHROMIUM
- Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium, 31-5
- Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethyldiammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S) tungstate(0), 587-92
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmethyl and dicarbonyl(dinitrogen)metal complexes, 651-6
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Magnetic susceptibility and optical spectra of the organic-intercalated two-dimensional ferromagnets bis(monomethylammonium)- and bis(monoethylammonium) tetrachlorochromate(II), 1207-12
- Chromium(II) chemistry. Part 12. Further examples of ferromagnetic chlorochromates(II), 1236-40
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- Crystal and molecular structure of di- μ -trimethylsilylmethyl-bis(trimethylphosphine)(trimethylsilylmethyl)chromium(II) (4Cr-Cr), 1314-18
- Decentralized unpaired electrons and valence bonding in chromium uranium trisulphide, 1686-90
- ### CLATHRATE
- X-ray crystallographic studies on ferrocene included in a thiourea host lattice, 15-18
- ### CLUSTER
- Carbon-13 nuclear magnetic resonance study of osmium complexes of the type $(\text{Os}_3(\text{CO})_9\text{H}(\text{X}))$, 196-8
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7

- Synthesis and molecular structure of bis(μ -but-1-yn-
-undecacarbonyl-quadro-tetrairon (4 Fe-Fe), 419-23
- New carbide clusters in the cobalt sub-group. Part 4. Synthesis
and crystallographic characterization of μ_3 -carbonyl-deca- μ -
carbonyl-dicarbido-tetradecacarbonyl-polyhedro-
dodecacarbonyl, 459-63
- New carbide clusters in the cobalt sub-group. Part 5.
Crystallographic characterization of deca- μ -carbonyl-carbido-
octacarbonyl-polyhedro-octacarbonyl(2-) in its
bis(benzyltrimethylammonium) salt, 463-7
- Protonation of the decavanadate(6-) ion: a vanadium-51 nuclear
magnetic resonance study, 503-6
- Nitrogen derivatives of iron carbonyls. Part 5. New routes in the
mechanism of reaction of dodecacarbonyl-triangulo-triiron with
nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)
- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
- Synthesis and crystal structure of heptacarbonyl- μ_3 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangulo-tri-
iron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a
metal-atom cluster, 552-6
- Carbon-13 nuclear magnetic resonance spectra of polynuclear
carbonyls of cobalt and rhodium, 626-34
- Reactions of strained organosilicon heterocycles with
nonacarbonyldiiron(0). Part 2. Preparation and reactions of
silaferracyclopentanes, 665-73
- The chemistry of polynuclear compounds. Part 30. Some reactions
of dodecacarbonyltetrahydrotetraosmium: the molecular and
crystal structure of trihydrido- μ_2 -iodo-cyclo-
tetrakis(tricarbonylosmium)(4Os-Os), 673-6
- Crystal structures of octacaeisium and octarubidium dicosaniobates
968-72
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Triosmium clusters derived from benzylamine and benzyl alcohol:
formation of a μ_3 -o-phenylene complex in the conversion of
benzyl alcohol into benzene, 1201-6
- Organosulphur-transition metal chemistry. Part 4. The isomerism
of μ -thio- and μ -seleno-bis(carbonyl(η -cyclopentadienyl)
ruthenium) complexes, 1260-9
- Crystal and molecular structure of tri- μ -chloro-
hexakis(trimethylsilylmethyl)-triangulo-trirhenium(III), 1334-7
- Trimethylsilyl derivatives for the study of silicate structures. Part 5.
Trimethylsilylation of diopase, 1342-9
- The chemistry of polynuclear compounds. Part 31. Synthesis of
undecacarbonylhydridotriosmate(1-) and its reaction with
octadecacarbonylhexaosmium to give a carboxylate-bridged
anionic enneaosmium species, 1358-63
- Heteronuclear cluster systems. Part 12. Synthesis of μ -
phenylphosphinediyl-bis(tetracarbonylcobalt) and 1,1,1,2,2,2,3,3,
3-nonacarbonyl- μ_3 -phenylphosphinediyl-triangulo-dicobaltiron
1385-7
- Heteronuclear cluster systems. Part 13. Synthesis of μ -
diphenylphosphido-bridged carbonylmetal complexes, and
crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3-hexacarbonyl-1,3;
2,3-bis- μ -diphenylphosphido-triangulo-tricobalt, 1387-92
- Studies on transition metal cyano complexes. Part 2.
Unsubstituted cyanorhenates, $(\text{Re}(\text{CN})_5)_n$, and cyanorhenates
with thio-, seleno-, and nitrosyl ligands, 1411-17
- Bis(tetrabutylammonium) tetrakis(benzenethiolato- μ_3 -
selenidoiron), an iron-selenium cubic cluster compound, 1423-5
- Formal Diels-Alder dimerization of cyclooctatetraene induced by
carbonylruthenium complexes, 1514-23
- Reactions of dodecacarbonyl-triangulo-triruthenium and
dodecacarbonyltetrahydrotetraruthenium with mixtures of
cyclic polyolefins, 1523-8
- Structures of binary carbonyls and related compounds. Part 1. A
new approach to fluxional behaviour, 1554-68
- Group 1B organometallic chemistry. Part 25. Crystal and
molecular structure of 1,2,3;1,4,5;2,3,6,4,5,6-tetrakis- μ_3 -2-
dimethylaminophenyl-2,5,3,4-bis- μ_2 -4-tolylethynyl-octahydro-
hexacopper(I), 1800-6
- CNDO
He(I) photoelectron spectra of tetracarbonyliron complexes of
Group 5 ligands and of olefinic ligands, 695-8
- Molecular structure of divinyl sulphone as studied by electron
diffraction, vibrational spectroscopy, and semiempirical CNDO/2
molecular-orbital calculations, 861-8
- COBALT
Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with
cobalt(II), nickel(II), and copper(II); X-ray structure
determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-
triazacyclododec-1-ene)nickel(II), 68-76
- Preparation and properties of new molybdenum-
ethylenediaminetetraacetato-complexes formed by the oxidation
of the molybdenum(III,II) dimer ($\text{Mo}_2(\text{O}_2\text{CMe})(\text{OH})_2(\text{EDTA}))$
-, 100-4
- Kinetics and mechanism of the reduction of thiocyanato-,
isothiocyanato, and azido-pentaamminecobalt(III) by
pentaammineaquaruthenium(II) in aqueous solutions, 148-51
- Magnetic properties of hexakis(pyridine N-oxide)cobalt(II)
perchlorate, 160-5
- Crystal and molecular structures of $(\text{NN}'-(2-(2'\text{-pyridyl})\text{ethyl})$
ethylenebis(salicylideneiminato))iron(II) and -cobalt(II)-ethanol
(1/1), 185-91
- Crystal and molecular structure of (dioxygen)($\text{NN}'-(2-(2'\text{-pyridyl})$
ethyl)ethylenebis(salicylideneiminato))cobalt-acetonitrile (1/1),
191-6
- Structural and mechanistic studies of coordination compounds.
Part 20. Preparation and base hydrolysis of some cobalt(III)
complexes of quadridentate macrocyclic amines, 216-21
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and
mechanism of carbonyl replacement in a
nonacarbonylthiodicobaltiron, 222-7
- New carbide clusters in the cobalt sub-group. Part 5.
Crystallographic characterization of deca- μ -carbonyl-carbido-
octacarbonyl-polyhedro-octacarbonyl(2-) in its
bis(benzyltrimethylammonium) salt, 463-7
- Crystal and molecular structure of hydrido(tetrahydroborato)
bis(tricyclohexylphosphine)nickel(II), 482-5
- Kinetics of base hydrolysis of cis-aminebromobis(ethylenediamine)
cobalt(III) complexes in aqueous solutions at 25°C, 556-60
- Carbon-13 nuclear magnetic resonance spectra of polynuclear
carbonyls of cobalt and rhodium, 626-34
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,
4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Complexes of pyrimidine-2-thione with some bivalent metal halides
of the first transition series, 880-4
- Complexes with sulphur and selenium donor ligands. Part 6.
Kinetics and mechanism of the reaction between 1,2-
bis(diphenylphosphino)ethane and tris(OO'-dimethyl
phosphorodithioato)cobalt(III), 950-5
- Complexes with sulphur and selenium donor ligands. Part 7. The
crystal and molecular structure of
bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- Crystal structure and absolute configuration of cobalt-doped α -
hexaaquazinc(II) selenate, 977-80
- Coordination bond properties in phthalocyaninatometal(II)
complexes. Part 1. Stereochemistry and bond properties in
bis(4-methylpyridine)phthalocyaninatometal(II)-4-
methylpyridine (1/2) (metal = cobalt or iron), 1018-24
- Base hydrolysis of amino-acid esters and amides in the
coordination sphere of cobalt(III). Part 3. Hydrolysis of methyl
and ethyl 4-aminobutanoate, 1046-51
- Crystal and molecular structure of trans-diazido(C-meso-5,12-
dimethyl-1,4,8,11-tetraazacyclotetradecane)cobalt(III) azide,
1131-4
- Structural and mechanistic studies of coordination compounds. 22.
Preparation and ligand-substitution kinetics of trans-
dihalogeno- and trans-halogenoisothiocyanato-cobalt(III)
complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-
tetra-azabicyclo(11.3.1)-heptadeca-1(17),2,11,13,15-pentane,
1180-5
- Spectroscopic investigation of copper(II) bovine carbonic anhydrase
and its inhibitor derivatives, 1269-73
- Cobalt metallacycles. Part 5. Synthesis of pyridines from nitriles
and acetylenes via cobaltacyclopentadienes, 1278-82
- Heteronuclear cluster systems. Part 12. Synthesis of μ -
phenylphosphinediyl-bis(tetracarbonylcobalt) and 1,1,1,2,2,2,3,3,
3-nonacarbonyl- μ_3 -phenylphosphinediyl-triangulo-dicobaltiron
1385-7
- Heteronuclear cluster systems. Part 13. Synthesis of μ -
diphenylphosphido-bridged carbonylmetal complexes, and
crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3-hexacarbonyl-1,3;
2,3-bis- μ -diphenylphosphido-triangulo-tricobalt, 1387-92
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with
carbonyls of manganese, iron, and cobalt, 1452-4
- Complexes with sulphur and selenium donor ligands. Part 8. Some
4-phenylthiosemicarbazone complexes of cobalt(II) and the
crystal structure of bis(acetone 4-phenylthiosemicarbazone)

- cobalt(II) bromide (green form), 1549-54
- Structures of binary carbonyls and related compounds. Part 1. A new approach to fluxional behaviour, 1554-68
- Spectroscopy and reactions of copper(II), nickel(II), and cobalt(III) compounds in molten nitrites, 1589-93
- Kinetic and isotopic studies on the reaction of nitrous acid with *cis*-chlorobis(ethylenediamine)(hydroxylamine)cobalt(III), 1634-7
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5
- Trans-influence of anionic, neutral, and bridging ligands on the nuclear magnetic resonance spectra of methyl- and fluorobenzyl-bis(dimethylglyoximate)rhodium(III) complexes. Some observations on bridge formation, 1807-13
- Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20
- COMPUTER PROGRAM**
- A damped nonlinear least-squares computer program (DALSFEK) for the evaluation of equilibrium constants from spectrophotometric and potentiometric data, 115-23
- A damped nonlinear least-squares computer program (DALSFRK) for the evaluation of reaction rate constants, 123-31
- Computer simulation of metal-ion equilibria in biofluids. Part 2. Formation constants for zinc(II)-citrate-cysteine binary and ternary complexes and improved models of low-molecular-weight zinc species in blood plasma, 1433-8
- COPPER**
- Resonance-Raman spectra of copper(II) and nickel(II) diethyldithiocarbamates, 53-6
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10
- Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53
- Crystal and molecular structure of the polymeric complex chloro(2,5-dithiahexane)copper(I), 416-18
- Single-crystal electron spin resonance and electronic spectra of bis(β -alaninato)copper(II) hexahydrate, 526-30
- A microcalorimetric study of the macrocyclic effect. Enthalpies of formation of copper(II) and zinc(II) complexes with some tetra-aza macrocyclic ligands in aqueous solution, 577-83
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Effect of mixed-ligand complex formation on the ionization of the pyrrole hydrogens of histamine and histidine, 964-8
- Structure and spectroscopic properties of bis(N-cyclohexyl-3-methoxysalicylideneiminato)copper(II), 1051-7
- Metal complexes of sesquidentate ligands derived from 3-ethoxymethylenepentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithiobis(o-phenyleneiminomethylidene)bis(pentane-2,4-dionato)(2-)) -nickel(II) and -copper(II), 1057-62
- Equilibria of complex formation between several bivalent metal ions and macrocyclic tri- and penta-amines, 1081-5
- Thermodynamic and spectroscopic properties of mixed complexes in aqueous solution. Copper(II) complexes of 2,2'-bipyridyl and dicarboxylic acids, 1090-4
- Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5
- Magnetic exchange in some polynuclear bis(azole) dihalogenocopper(II) complexes, 1170-5
- Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, 1269-73
- The isomers of α -amino-acids with copper(II). Part 4. Catalysis of the racemization of optically active alanine by copper(II) and pyruvate in alkaline solution, 1444-7
- Spectroscopy and reactions of copper(II), nickel(II), and cobalt(III) compounds in molten nitrites, 1589-93
- Crystal and molecular structure and magnetic properties of tetrakis(2-diethylaminoethanolato)isocyanatocopper(II), 1594-8
- Reactions between copper(II) and 2-mercaptosuccinic acid in aqueous perchlorate solution, 1606-9
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- Group 1B organometallic chemistry. Part 25. Crystal and molecular structure of 1,2,3,1,4,5,2,3,6,4,5,6-tetrakis- μ_3 -2-dimethylaminophenyl-2,5,3,4-bis- μ_2 -4-tolylethynyl-octahedro-hexacopper(I), 1800-6
- CROWN ETHER**
- Complexes of lanthanoid salts with the crown ether *cis*,*syn*,*cis*-2,5,8,15,18,21-hexaoxatricyclo(20.4.0.0^{9,14})hexacosane and their paramagnetically shifted nuclear magnetic resonance spectra, 181-4
- Ligands for the alkali metals. Part 4. Nuclear magnetic resonance of crown ethers with alkali-metal ions, 611-17
- Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- CRYSTAL**
- A potentially seven-coordinate complex that is only five-coordinate; crystal and molecular structure of di-iodo(6,7,8,9-tetrahydro-16,22-dimethyl-5,10-dithia-15,23,24-triaza-17,21-methenodibenzo(a,i)cyclononadecene-NN'N'')zinc(II), 511-16
- Metal complexes of sesquidentate ligands derived from 3-ethoxymethylenepentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithiobis(o-phenyleneiminomethylidene)bis(pentane-2,4-dionato)(2-)) -nickel(II) and -copper(II), 1057-62
- CRYSTAL STRUCTURE**
- X-ray crystallographic studies on ferrocene included in a thiourea host lattice, 15-18
- Preparation and structure of 1,4-dichloro-1,1,3,3-tetraphenylcatena-di(boraphosphane), BH₂Cl.PPh₂.BH₂Cl.PPh₂Cl, 40-3
- Unsaturated σ -hydrocarbyl transition-metal complexes. Part 4. Crystal and molecular structure of trans-chlorobis(diethylphenylphosphine)(phenylethynyl)platinum(II) and comments on the relative trans influence of various carbon ligands, 46-50
- Crystal structure of abode-pentacarbonyl-f- μ -fluoro-ghijk-pentafluororhenium(II)rhenium(V), 64-7
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- Ruthenium complexes containing Group 5B donor ligands. Part 5. Synthesis and crystal and molecular structure of acetone(carbonyl)chloro(trichlorostannio) bis(triphenylphosphine)ruthenium(II)-acetone (1/1), 76-9
- Crystal and molecular structure and some properties of pyridinium μ -oxobis(trichloroferrate(III))-pyridine, 80-4
- Coordinative tin-oxygen interactions in dinitratodiphenyl(triphenylphosphine oxide)tin(IV), 131-3
- Crystal and molecular structures of (η -methylcyclopentadienyl)(η -7-exophenylcyclohepta-1,3,5-triene)manganese, 144-7
- Crystal and molecular structures of (NN'-(2-(2'-pyridyl)ethyl) ethylenebis(salicylideneiminato))iron(II) and -cobalt(II)-ethanol (1/1), 185-91
- Crystal and molecular structure of (dioxigen)(NN'-(2-(2'-pyridyl) ethyl)ethylenebis(salicylideneiminato))cobalt-acetonitrile (1/1), 191-6
- Structural studies of steric effects in phosphine complexes. Part 3. The synthesis, characterization and molecular structure of diacetato(tris(tert-butyl)phosphine)mercury(II), 253-6
- Synthesis and crystal structure of 3,3,4-tricyano-2,2-bis(triphenylphosphine)-1-oxa-2-platinacyclobutane, 279-82
- Structure of (η -allyl)dicarbonyl(pentane-2,4-dionato)pyridinemolybdenum(II) in the solid and solution states, 291-5
- Carborane derivatives of the late- and post-transition elements. Part 1. Preparation and X-ray crystal structure of 3-diethyldithiocarbamato-1,2-dicarba-3-auradodecaborane(II), 303-9
- Rhodium(I) complexes of diallyl ethers and related compounds, 333-9
- Carbonyltrichlorotris(dimethylphenylphosphine)technetium-ethanol (1/1), the first seven-coordinate complex of technetium; position of this molecule in the C_{3v} family, 373-80

- Comparison of the different modes of bonding of the macrocycle in μ -(1,4,8,11-tetrathiacyclotetradecane-Si⁴⁺S⁸S¹¹)
-bis(dichloromercury(II)) and aqua(1,4,8,11-tetrathiacyclotetradecane)mercury(II) perchlorate by X-ray structural analysis, 394-9
- Hydrocarbon complexes of iron, ruthenium, and osmium. 11.
Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3-6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
- Crystal and molecular structure of μ -pentalenebis(dicarbonyl(trimethylgermyl)ruthenium), 412-16
- Crystal and molecular structure of the polymeric complex chloro(2,5-dithiahexane)copper(I), 416-18
- Synthesis and molecular structure of bis(μ -but-1-yne)-undecacarbonyl-quattro-tetrairon (4 Fe-Fe), 419-23
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- New carbide clusters in the cobalt sub-group. Part 4. Synthesis and crystallographic characterization of μ_3 -carbonyl-deca- μ -carbonyl-dicarbido-tetradecacarbonyl-polyhedro-dodecacarbonyl, 459-63
- New carbide clusters in the cobalt sub-group. Part 5. Crystallographic characterization of deca- μ -carbonyl-carbido-octacarbonyl-polyhedro-octacobaltate(2-) in its bis(benzyltrimethylammonium) salt, 463-7
- Crystal and molecular structure of hydrido(tetrahydroborato)bis(tricyclohexylphosphine)nickel(II), 482-5
- Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
- Preparations and structures of NN'
-ethylenebis(salicylideneiminato)titanium(III) derivatives, 545-9
- Synthesis and crystal structure of heptacarbonyl- μ_3 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangulo-triiron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a metal-atom cluster, 552-6
- The crystal structure of tin(II) bis(dihydrogenphosphate), 566-9
- X-ray crystal structures of μ_4 -chloro-(tris(trichloro(thiosemicarbazide)bismuth(III)))
(tris(thiosemicarbazide)bismuth(III)) hexachlorobismuthate(III) chloride and catena- μ -chloro-dichlorobis(ethylenethiourea) bismuth(III), 583-7
- Unidentate sulphur-bonded monothio- β -diketon complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
- The chemistry of uranium. Part 20. Tetraphenylphosphonium pentachloro-oxouranate(IV): crystal structure and bonding characteristics, 592-7
- Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601
- Trimethylphosphine oxide complexes of thorium and uranium tetranitrates; crystal structures of ten- and twelve-coordinate complex ions, bis(trinitratotetrakis(trimethylphosphine oxide)thorium(IV)) hexanitratothorate(IV) and tetraphenylphosphonium pentanitrato-bis(trimethylphosphine oxide)thorate(IV), 638-46
- Crystal and molecular structure of NN-di-isopropyl-P-phenylphosphonamidic chloride, PPh(Cl)(NPr₂)O, 647-50
- The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyl-tetrahydridotetraosmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-tetrakis(tricarbonylosmium)(4Os-Os), 673-6
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Metal complexes of sulphur ligands. 16. Reaction of trichlorotris(dimethylphenylphosphine)ruthenium and dichlorotris(triphenylphosphine)ruthenium with sodium and ammonium monothiobenzoates; structure of (4-amino-2-imino-4-methylpentane)bis(dimethylphenylphosphine)bis(monothiobenzoato)ruthenium(II), 769-75
- Nitrosyl complexes of rhenium. Part 3. Crystal and molecular structure of tetraethylammonium tetrachloronitrosyl(pyridine) rhenate(1-), 798-801
- Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine)diplatinum complexes: crystal and molecular structure of di- μ -hydridobis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
- Preparation, properties, and crystal structure of tetraethylammonium bis(1,3-diphenylpropane-1,3-dionato)nitratodioxouranate(VI), 818-21
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Structural studies of nitrido-complexes: X-ray crystal structure of tetraphenylarsonium pentakis(isothiocyanato)nitridorhenate(VI), 844-8
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-o-tolyl phosphite iridium(III) complexes, 926-31
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Reactions of tellurium: oxides with alkali-metal oxides and hydroxides, 948-50
- Complexes with sulphur and selenium donor ligands. Part 7. The crystal and molecular structure of cobalt
bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- Crystal structures of octa- and octarubidium dicosaniobates 968-72
- Crystal structure and absolute configuration of cobalt-doped α -hexa-aquazinc(II) selenate, 977-80
- Structural studies on biguanide and related species. Correlation of protonation energy with molecular structure, 989-96
- Coordination bond properties in phthalocyaninatometal(II) complexes. Part 1. Stereochemistry and bond properties in bis(4-methylpyridine)phthalocyaninatometal(II)-4-methylpyridine(1/2) (metal = cobalt or iron), 1018-24
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine) ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- Structural studies of substituted hydrazine complexes. Part 2. Crystal and molecular structure of (η -cycloocta-1,5-diene)tris(NN-dimethylhydrazine)hydridoruthenium(II) hexafluorophosphate, 1040-2
- Structural studies of substituted hydrazine complexes. Part 3. Crystal and molecular structure of dichlorobis(η -cycloocta-1,5-diene)(NN-dimethylhydrazine)dihydridodiruthenium, an asymmetric triply bridged dimer containing a bidentate bridging NN-dimethylhydrazine ligand, 1043-6
- Structure and spectroscopic properties of bis(N-cyclohexyl-3-methoxysalicylideneiminato)copper(II), 1051-7
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from MoMe(CO)₂(η -C₃H₃) and but-2-yne, 1067-80
- Crystal structure of 2,trans-4,cis-6,trans-8-tetrachloro-2,4,6,8-tetrakis(dimethylamino)cyclooctaphosphazene, 1094-8
- Some mononuclear seven-coordinate rhenium(III) carbonyl complexes; the crystal and molecular structure of (2,2-bipyridyl)tribromodicarbonylrhenium(III), 1098-102
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxo-OP)(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)-C¹PO₂(methyl isocyanide)iridium(III), 1119-26
- Crystal and molecular structure of trans-diazido(C-meso-5,12-dimethyl-1,4,8,11-tetraazacyclotetradecane)cobalt(III) azide, 1131-4
- Platinum hydrides containing silyl or germyl ligands. Crystal structure of trans-hydridosilylbis(tricyclohexylphosphine)platinum(II), 1167-70

- Crystal and molecular structure of trichloro(2,5,8-trioxanonane) titanium(III), 1176-9
- Crystal and molecular structure of di- μ -bromo- μ -tetraphenyldiphosphane-bis(tricarbonylrhenium(I)), 1189-95
- Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine)tris(isothiocyanato)rhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio) methanethiolato-bis(tricarbonylmanganese), 1247-55
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- Derivatives of bivalent germanium, tin, and lead. Part 21. Tin(II) formate: a reinvestigation, 1274-8
- Comparison of the structure and dynamic properties of anion(1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) perchlorate complexes in nitromethane solutions, and the crystal and molecular structure of the chloro complex, 1282-8
- Crystal and molecular structure of di- μ -trimethylsilylmethyl-bis(trimethylphosphine)(trimethylsilylmethyl)chromium(II) (4Cr-Cr), 1314-18
- Crystal structures of methyl(l-tyrosinato)mercury(II) monohydrate and (l-(2-amino-4-phenylbutanoato))methylmercury(II), 1324-8
- Crystal and molecular structure of tri- μ -chloro-hexakis(trimethylsilylmethyl)-triangulo-trirhenium(III), 1334-7
- Single-crystal molecular and electronic structure of trichlorooxo(triphenylphosphine sulphide)molybdenum(V), 1350-4
- Molecular and crystal structure of 3,3-bis(triethylphosphine)-1,2-dicarba-3-platinadodecaborane(11), and molecular orbital analysis of the slip distortion in carbametallaboranes, 1363-74
- Reactions of metal carbonyl derivatives. Part 22. The crystal and molecular structures of dicarbonyl(η -cyclopentadienyl)(ethylthio) iron and μ -ethylthio-bis(dicarbonyl(η -cyclopentadienyl)iron) tetrafluoroborate, and a comparison of their molecular parameters, 1379-85
- Heteronuclear cluster systems. Part 13. Synthesis of μ -diphenylphosphido-bridged carbonylmetal complexes, and crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3-hexacarbonyl-1,3; 2,3-bis- μ -diphenylphosphido-triangulo-tricobalt, 1387-92
- Addition reactions on coordinated olefinic ligands. Part 8. Platinum(II) complexes of 1,1-dimethylallene and their reaction with amines. Molecular structure of the zwitterionic derivative dichloro(1-(NN-diethylammoniomethyl)-2-methylprop-1-enyl)(triphenylphosphine)platinum(II), 1392-7
- Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403
- Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodiimide (cyanamide), 1407-11
- Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaaxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- Crystal structure of compounds with (N-P)_n rings. Part 12. Decafluorocyclopentaphosphazene, 1425-30
- Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropenone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
- Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl-N)palladium(II) perchlorate, 1490-6
- Crystal structure of dilead tritellurate(IV), 1528-32
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine) molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Crystal structure of tetrakis- μ -trifluoroacetato-bis(triaqua(trifluoroacetato)praseodymium(III)), 1544-8
- Complexes with sulphur and selenium donor ligands. Part 8. Some 4-phenylthiosemicarbazone complexes of cobalt(II) and the crystal structure of bis(acetone 4-phenylthiosemicarbazone) cobalt(II) bromide (green form), 1549-54
- Crystal structure of exo-6-chloromercurio-6,7-dihydro-exo-7-methoxyaldrin (1,2,3,4,10,10-hexachloro-exo-6-chloromercurio-1,4,4a,5,6,7,8,8a-octahydro-endo,exo-1,4:5,8-dimethano-exo-7-methoxynaphthalene), 1573-6
- Studies in eight-coordination. Part 5. Crystal and molecular structure and electron spin resonance spectra of tetrakis(diethylthiocarbamate)molybdenum(V) hexamolybdate and chloride, 158_-9
- Crystal and molecular structure and magnetic properties of tetrakis(2-diethylaminoethanolato)isocyanatocopper(II), 1594-8
- Rhenium carbonyl fluorides: preparation, crystal structure, and some properties of hexacarbonylrhenium(I) μ -fluoro-bis(pentafluororhenate(V)), 1627-31
- Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (-)-578-carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino) diphenylphosphine)nitrosylmolybdenum, 1664-70
- Structure and properties of cis-bis(dicyclohexylphosphine) dihalogenonickel(II) complexes, 1671-7
- Crystal structure of trichlorosulphonium(IV) tetrachloroiodate(III), 1723-5
- Carbonylhalogeno(o-phenylenebis(dimethylarsine))osmium complexes including those containing unidentate o-phenylenebis(dimethylarsine), 1726-32
- The structure of tin(II) thiocyanate, 1797-9
- Group 1B organometallic chemistry. Part 25. Crystal and molecular structure of 1,2,3;1,4,5;2,3,6;4,5,6-tetrakis- μ_3 -2-dimethylaminophenyl-4,3-bis- μ_2 -4-tolylethynyl-octahydro-hexacopper(I), 1800-6
- Crystal and molecular structure of (Pd₃(C₃Ph(p-MeOC₆H₄)₂)₂(acac)₂), derived from a triarylcyclopropenium salt and a palladium(0) complex, 1825-30
- Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine) (1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47
- Crystal and molecular structure and electron spin resonance spectrum of trichlorooxo-bis(triphenylphosphine oxide) molybdenum(V), 1848-54
- ### CYANIDE
- Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7
- Kinetics and mechanism of replacements in pentacyano(ligand) ferrate(II) ions. An attempt to distinguish between the D and I_d mechanisms, 500-2
- Nuclear magnetic resonance studies of the addition of hydrogen halides to trans-cyanohydrido-bis(triethylphosphine)platinum(II) and hydridotris(triethylphosphine)platinum(II) tetraphenylborate, 877-9
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6. The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- Studies on transition metal cyano complexes. Part 2. Unsubstituted cyanorhenates, (Re(CN)₅)₂²⁻, and cyanorhenates with thio-, seleno-, and nitroso ligands, 1411-17
- Kinetics and mechanisms of formation, and of reactions, of intermediates in the iron(II)-1,10-phenanthroline-cyanide and related systems, 1447-51
- Solution effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6
- Kinetics of reaction of imidazole, glycine, and L-histidine with the aquapentacyanoferrate(II) ion, 1610-17
- ### CYCLOCONDENSATION
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- ### CYCLOHEPTATRIENE
- Crystal and molecular structures of (η -methylcyclopentadienyl)(η -7-exophenylcyclohepta-1,3,5-triene)manganese, 144-7

CYCLOOCTADIENE

- Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14
- Preparation of (η -cycloocta-1,5-diene) halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
- Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine) ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9
- Structural studies of substituted hydrazine complexes. Part 2. Crystal and molecular structure of (η -cycloocta-1,5-diene)tris(NN-dimethylhydrazine)hydridoruthenium(II) hexafluorophosphate, 1040-2
- Structural studies of substituted hydrazine complexes. Part 3. Crystal and molecular structure of dichlorobis(η -cycloocta-1,5-diene)(NN-dimethylhydrazine)dihydridoruthenium, an asymmetric triply bridged dimer containing a bidentate bridging NN-dimethylhydrazine ligand, 1043-6
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- Use of aryltin compounds in the preparation of diaryl- and diaroyle-d μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of $(M(C_5Me_5)(sol)_3)(PF_6)_2$ ($M = Rh$ or Ir ; $sol = MeCN, Me_2CO$, or $MeOH$) with mono-, di-, and triolefins, 1305-11
- Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropenone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediyldiene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
- Binuclear diaryltriazenido- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
- The preparation, structures, and reactions of the metallocyclobutenyl complexes $(M_3(C_3R^1R^2)_2X_2)$ derived from addition of triarylcyclopropenone salts to zerovalent palladium and platinum compounds, 1830-9
- Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47

CYCLOOCTATETRAENE

- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^4 -cyclooctatetraene)(1-6- η^6 -cyclooctatetraene)iron, 1761-6

CYCLOOCTATRIENE

- Hydrocarbon complexes of iron, ruthenium, and osmium. 11. Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3:6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12

CYCLOPENTADIENYL

- Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium, 31-5
- Electron spin resonance studies of Ziegler-type catalysts. Part 2. Identification and spectra of some dialkylidene(η -cyclopentadienyl)vanadium(IV) complexes, 57-61
- Crystal and molecular structures of (η -methylcyclopentadienyl)(η -7-exophenylcyclohepta-1,3,5-triene)manganese, 144-7
- Some oxygen-donor complexes of cyclopentadienyluranium(IV) halides, 295-8

Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33

The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 7. The fluxional behaviour of bis(cyclopentadienyl)dithiocarbamatomolybdenum complexes, and the application of Forsen-Hoffman spin-saturation method to the nuclear magnetic resonance spectra of a five-spin system, 467-74

The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9

The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2

Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95

Synthesis and crystal structure of heptacarbonyl- μ_3 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangular-iron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a metal-atom cluster, 552-6

The quenching of excited uranyl ion by d^6 metallocenes, 569-72

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26

Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34

Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6

The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57

Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7

Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43

Formation of η^3 -bonded lactone complexes and eight-membered ring metallocycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $MoMe(CO)_3(\eta-C_3H_3)$ and but-2-yne, 1067-80

An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonylbis(η -dienyl)isocyanidediiron complexes, 1185-9

Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6

Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio) methanethiolato-bis(tricarbonylmanganese), 1247-55

Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60

Organosulphur-transition metal chemistry. Part 4. The isomerism of μ -thio- and μ -seleno-bis(carbonyl(η -cyclopentadienyl) ruthenium) complexes, 1260-9

Cobalt metallocycles. Part 5. Synthesis of pyridines from nitriles and acetylenes via cobaltacyclopentadienes, 1278-82

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of $(M(C_5Me_5)(sol)_3)(PF_6)_2$ ($M = Rh$ or Ir ; $sol = MeCN, Me_2CO$, or $MeOH$) with mono-, di-, and triolefins, 1305-11

Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di- μ -arythio-bis(η -cyclopentadienyl)rhodium, 1375-9

Reactions of metal carbonyl derivatives. Part 22. The crystal and molecular structures of dicarbonyl(η -cyclopentadienyl)(ethylthio) iron and μ -ethylthio-bis(dicarbonyl(η -cyclopentadienyl)iron) tetrafluoroborate, and a comparison of their molecular

- parameters, 1379-85
- Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403
- Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14
- Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (η -578-carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino)diphenylphosphine)nitrosylmolybdenum, 1664-70
- The preparation, structures, and reactions of the metallacyclobutenyl complexes ($M_2(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- CYCLOPHOSPHAZENE**
- Organosubstituted phosphazenes. Part 9. Mass spectra of phenyl-substituted chlorocyclophosphazenes, 173-7
- CYSTEINE**
- Gold complexes of L-cysteine and D-penicillamine, 199-201
- DIAZENIDE**
- Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in aryl diazenidotris(dimethyldithiocarbamate)molybdenum, 1654-8
- DICARBOXYLATE**
- Reactions between copper(II) and 2-mercaptosuccinic acid in aqueous perchlorate solution, 1606-9
- DIELS ALDER**
- The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2
- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- DIENE**
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine)ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- DIKETONATE**
- Structure of (η -allyl)dicarbonyl(pentane-2,4-dionato)pyridinemolybdenum(II) in the solid and solution states, 291-5
- Nuclear magnetic resonance studies of lanthanoid complexes. Part 3. Adducts of tris(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctane-3,5-dionato)praseodymium with bidentate amines, 315-19
- Rhodium(I) complexes of diallyl ethers and related compounds, 333-9
- Standard enthalpies of formation of tris(bis(pentane-2,4-dionato)nickel(II)) and bis(2,2,6,6-tetramethylheptane-3,5-dionato)nickel(II) and an estimation of nickel-oxygen bond energies, 399-402
- Electron spin resonance spectra of trigonal-prismatic bis(pentane-2,4-dione benzoylhydrazonato(2-))vanadium(IV) and bis(4-phenylbutane-2,4-dione benzoylhydrazonato(2-))vanadium(IV), 423-6
- Chemistry of polydentate ligands. Part 3. Ring closures effected by the reaction of β -diketones with 6,6'-dihydrazino- and 6,6'-di-(N-methylhydrazino)-2,2'-bipyridylnickel(II) diperchlorate, 440-6
- Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
- Preparation, properties, and crystal structure of tetraethylammonium bis(1,3-diphenylpropane-1,3-dionato)nitratodioxouranate(VI), 818-21
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Metal complexes of oxidant ligands derived from 3-ethoxymethylene-pentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithiobis(o-phenyleneiminomethylidene))bis(pentane-2,4-dionato(2-))nickel(II) and -copper(II), 1057-62
- The standard enthalpies of formation of tris(pentane-2,4-dionato)molybdenum(III) and dioxobis(pentane-2,4-dionato)molybdenum(VI), and the molybdenum-pentane-2,4-dionate bond-enthalpy contributions, 1311-13
- Preparation and physicochemical characterization of anionic uranyl β -ketoenolates, 1618-21
- Crystal and molecular structure of $(Pd_3(C_3Ph(p-MeOC_6H_4)_2)_2(acac)_2)$, derived from a triarylcyclopropenium salt and a palladium(0) complex, 1825-30
- The preparation, structures, and reactions of the metallacyclobutenyl complexes ($M_2(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- DIKETONE**
- The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9
- DIOPTASE**
- Trimethylsilyl derivatives for the study of silicate structures. Part 5. Trimethylsilylation of diopase, 1342-9
- DIPHOSPHORUS**
- Multinuclear magnetic resonance studies. Part 3. Compounds with phosphorus-oxygen-phosphorus or phosphorus-sulphur-phosphorus bridges, 9-12
- DIPOLE MOMENT**
- Preparation and structures of ruthenium(III) complexes containing tertiary arsines, tertiary phosphines, and isocyanides, 1152-4
- DITHIOACID**
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- Metal complexes of sulphur ligands. Part 18. Reaction of tri- and tetraakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- DITHIOCARBAMATE**
- Carbaborane derivatives of the late- and post-transition elements. Part 1. Preparation and X-ray crystal structure of 3-diethyldithiocarbamate-1,2-dicarba-3-aurododecaborane(11), 303-9
- DITHIOPHOSPHATE**
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- Complexes with sulphur and selenium donor ligands. Part 6. Kinetics and mechanism of the reaction between 1,2-bis(diphenylphosphino)ethane and tris(OO'-dimethylphosphorodithioato)cobalt(III), 950-5
- Complexes with sulphur and selenium donor ligands. Part 7. The crystal and molecular structure of bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- DMSO**
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- Axial ligand dissociation of phthalocyaninatoiron(II) adducts. Further evidence for a dissociative mechanism of substitution, 1709-14
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide)aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- DOPA**
- Assignment of the proton-association constants for 3-(3,4-dihydroxyphenyl)alanine (L-dopa), 43-5
- EDTA**
- Preparation and characterization of dimeric molybdenum(III)-ethylenediaminetetraacetate complexes, 95-9
- Preparation and properties of new molybdenum-ethylenediaminetetraacetato-complexes formed by the oxidation of the molybdenum(III,III) dimer ($Mo_2(O_2CMe)(OH)_2(EDTA)$), 100-4
- Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53
- Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
- ELECTROCHEM**
- Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
- Preparation, structure, and redox properties of isocyanide

- complexes of molybdenum(0) and tungsten(0), 165-9
 Thermodynamics of metal complex formation in aqueous melts of calcium dinitrate-ammonium nitrate. Part 2. Cadmium(II) bromides, 549-52
 Mixed-ligand complexes of palladium(II). Part 3. Diaqua(ethylenediamine)palladium(II) complexes of L-amino acids, 726-8
 Reaction of electrogenerated square-planar nickel(I) complexes with alkyl halides, 972-6
 Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine)trisothiocyanatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
 Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti- μ -arylythio-bis(η -cyclopentadienyl)rhodium), 1375-9
 Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- ELECTROLYSIS**
 Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
- ELECTRON DIFFRACTION**
 Electron-diffraction investigation of the molecular structure of sulphonyl chloride isocyanate, 299-302
 Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8
- ELECTRONIC STRUCTURE**
 A molecular-orbital evaluation of skeletal electron-counting procedures, 18-25
 Effects of extra hydrogens on the electronic structures of five- and six-vertexed polyhedral boranes, 25-31
- ENZYME**
 Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, 1269-73
- EPIMERIZATION**
 Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino acids, 152-8
- ESR**
 Electron spin resonance studies of Ziegler-type catalysts. Part 2. Identification and spectra of some dialkyldi(η -cyclopentadienyl)vanadium(IV) complexes, 57-61
 Photochemical studies of the alkylammonium molybdates. Part 4. Electron spin resonance study of an irradiated single crystal of hexakis(isopropylammonium) dihydrogen octamolybdate dihydrate, 283-5
 Electron spin resonance spectra of trigonal-prismatic bis(pentane-2,4-dione benzoylhydrazonato(2-))vanadium(IV) and bis(4-phenylbutane-2,4-dione benzoylhydrazonato(2-))vanadium(IV), 423-6
 Reactions of dichlorodiphenoxotitanium(IV), 454-9
 Single-crystal electron spin resonance and electronic spectra of bis(β -alaninato)copper(II) hexahydrate, 526-30
 Sulphur-nitrogen compounds. Part 5. The oxidation of N-aryl-N-(arylsulphonyl)hydroxylamines: preparation of N-aryl-NO-bis(arylsulphonyl)hydroxylamines, 604-7
 Low-temperature magnetic studies of a linear trimeric nickel compound: abcjkl-hexa-aqua-def:ghi-hexakis(μ -1,2,4-triazole- N_1N_2)-trinickel(II) hexanitrate dihydrate, 702-4
 Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
 Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
 Thermodynamic and spectroscopic properties of mixed complexes in aqueous solution. Copper(II) complexes of 2,2'-bipyridyl and dicarboxylic acids, 1090-4
 Magnetic exchange in some polynuclear bis(azole) dihalogenocopper(II) complexes, 1170-5
 Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, 1269-73
 Metal complexes of uridine and thymidine, 1294-7
 Single-crystal molecular and electronic structure of trichlorooxo(triphenylphosphine sulphide)molybdenum(V), 1350-4
 Studies in eight-coordination. Part 5. Crystal and molecular structure and electron spin resonance spectra of tetrakis(diethyldithiocarbamate)molybdenum(V) hexamolybdate and chloride, 1582-9
 Reactions between copper(II) and 2-mercaptosuccinic acid in aqueous perchlorate solution, 1606-9
 Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
 Versatility of the coordination behaviour of 1-methylpyrimidine-2-thione towards metal ions of the first transition series, 1705-9
 Crystal and molecular structure and electron spin resonance spectrum of trichlorooxobis(triphenylphosphine oxide)molybdenum(V), 1848-54
- ETHER**
 Rhodium(I) complexes of diallyl ethers and related compounds, 333-9
 Dealkylation of chelating ethers by reaction with WCl_4Y ($Y = O, S, Se, \text{ or } NC_2Cl_3$), 1658-61
- ETHYLENE**
 Reactions of platinum(II) complexes. Part 2. Catalysis of the aquation of tetrachloroplatinate(II) ion by trichloro(η -ethylene)platinate(II) (Zeise's anion), 158-9
- EUTECTIC**
 Spectroscopy and reactions of copper(II), nickel(II), and cobalt(III) compounds in molten nitrites, 1589-93
- EXCHANGE**
 Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino acids, 152-8
 Carbon-13 nuclear magnetic resonance study of osmium complexes of the type $(Os_3(CO)_9H(X))$, 196-8
 Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7
 Nuclear magnetic resonance studies of lanthanoid complexes. Part 3. Adducts of tris(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctane-3,5-dionato)praseodymium with bidentate amines, 315-19
 Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
 Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
 Reactions of bis(trifluoromethyl)mercury: the synthesis and properties of methyl(trifluoromethyl)-stannanes and -plumbanes 541-4
 Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
 Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
 Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
 Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxo-OP)(2-((2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanato(2-)-C¹PO₂)(methyl isocyanide)iridium(III), 1119-26
 Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
 Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
 Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in arylidiazeneidotrakis(dimethyldithiocarbamate)molybdenum, 1654-8
 Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5
 A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^4 -cyclooctatetraene)(1-6- η^6 -cyclooctatetraene)iron, 1761-6
 Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide)aluminium(III) ion with unl^- , bi^- , and ter -dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- EXTN EQUIL**
 Thermodynamics of extraction equilibria. Part 5. Correction of the method for the determination of equilibrium constants of extraction processes, 1-4

FERROCENE

X-ray crystallographic studies on ferrocene included in a thiourea host lattice, 15-18

FLUORIDE

Crystal structure of *abede*-pentacarbonyl-*f-μ*-fluoro-*ghijk*-

pentafuororhenium(I)rhenium(V), 64-7

Vapour-phase intensity studies of the Raman-active bands of

Group 6 hexafluorides, 170-3

Co-condensation reactions of uranium tetrafluoride and hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40

Rhenium carbonyl fluorides: preparation, crystal structure, and some properties of hexacarbonylrhenium(I) *μ*-fluoro-bis(pentafluororhenate(V)), 1627-31

FLUORITE

A structural theory for nonstoichiometry. Part 4. Defect fluorite-type structures: vacancy superstructures in ordered calcium oxide-hafnium dioxide ternary oxides, 320-8

FORCE CONST

Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5

Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6

Molecular vibrations of zirconium(IV) tetrahydroborate, a compound containing triple hydrogen bridges, 710-22

Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8

Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy, 921-5

The structure of ac-dichloro-*b*-ethylene-*d*-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8

GADOLINIUM

The gadolinium-hydrogen system, 601-4

GALLIUM

Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17

GERMANIUM

Hydrocarbon complexes of iron, ruthenium, and osmium. 11.

Diruthenium complexes of pentadiene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3:6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentadiene precursor, 403-12

Crystal and molecular structure of *μ*-pentadienebis(dicarbonyl(trimethylgermyl)ruthenium), 412-16

Transition-metal carbonyl derivatives of the germanes. Part 6. The methylgermyl iron carbonyl system, 506-11

Transition-metal carbonyl derivatives of the germanes. Part 7.

Properties of complexes containing dimethylgermyliron carbonyl groups and their interconversion, 722-6

Preparation and properties of some silyl- and germlyl-

halogenoacetylenes and of digermylacetylene, 759-63

Platinum hydrides containing silyl or germlyl ligands. Crystal structure of trans-hydridosilylbis(tricyclohexylphosphine) platinum(II), 1167-70

Transition-metal carbonyl derivatives of the germanes. Part 9.

Reactions of tetracarbonyldi(methylgermyl)iron with some covalent halides, 1569-73

Transition-metal carbonyl derivatives of the germanes. Part 10.

Tetracarbonyldigermanylcobalt, 1752-5

GOLD

Gold complexes of L-cysteine and D-penicillamine, 199-201

Carbaborane derivatives of the late- and post-transition elements.

Part 1. Preparation and X-ray crystal structure of 3-diethyldithiocarbamate-1,2-dicarba-3-aurodecaborane(11), 303-9

Kinetics of oxidation of dichlorobis(substituted pyridine) platinum(II) and of reduction of tetrachlorobis(substituted pyridine)platinum(IV) complexes, 699-702

Displacement of chelate ligands from planar four-coordinate complexes. Part 5. Preparation and ligand-substitution reaction of dichloro(ethylenediamine)- and dichloro(propylenediamine)-

-gold(III) complexes, 728-34

Reactions of hexafluorobut-2-yne with alkylgold(I) complexes.

Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5

Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5

GRIGNARD REAGENT

Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14

GROUP IB

Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5

GROUP II

Soft-sphere ionic radii for Group 1 and Group 2 metal halides and ammonium halides, 1631-4

GROUP IIB

Equilibria of complex formation between several bivalent metal ions and macrocyclic tri- and penta-amines, 1081-5

Thermochemistry of dichlorobis(triphenylphosphine oxide)-zinc(II)-cadmium(II), and -mercury(II), 1102-4

GROUP VB

He(I) photoelectron spectra of tetracarbonyliron complexes of Group 5 ligands and of olefinic ligands, 695-8

GROUP VIA

Vapour-phase intensity studies of the Raman-active bands of Group 6 hexafluorides, 170-3

Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(II), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56

Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53

Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92

GROUP VIB

Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7

GROUP VII

Metal complexes of uridine and thymidine, 1294-7

GROUP VIIA

Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(II), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56

GROUP VIII

Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80

Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(II), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56

Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53

Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44

Tetramethylthiophen complexes of rhodium, iridium, palladium,

- and ruthenium, 857-61
- Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Structures of binary carbonyls and related compounds. Part 1. A new approach to fluxional behaviour, 1554-68
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- HAFNIUM**
- A structural theory for nonstoichiometry. Part 4. Defect fluorite-type structures: vacancy superstructures in ordered calcium oxide-hafnium dioxide ternary oxides, 320-8
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Photoelectron spectra of metal tetrahydroborates, 1755-61
- HEMIMORPHITE**
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- HETEROCYCLE**
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- $^5\text{T}_2\text{-A}_1$ transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- Reactions of strained organosilicon heterocycles with nonacarbonyliron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Low-temperature magnetic studies of a linear trimeric nickel compound: abcdjkl-hexa-aqua-def.ghi-hexakis(μ -1,2,4-triazole- $\text{N}(\text{N}2)$ -triricel(II) hexanitrile dihydrate, 702-4
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Tetramethylthiophen complexes of rhodium, iridium, palladium, and ruthenium, 857-61
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Complexes of platinum(II) with 2,2'-bipyrimidine: the effect of hydrogen bonding on intermetallic interactions, 1127-30
- Magnetic exchange in some polynuclear bis(azole) dihalogenocopper(II) complexes, 1170-5
- Metal complexes of uridine and thymidine, 1294-7
- Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl)-N)palladium(II) perchlorate, 1490-6
- Dynamic behaviour in solution of some benzo(h)quinoline and 8-methylquinoline complexes of palladium(II), 1497-501
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- Versatility of the coordination behaviour of 1-methylpyrimidine-2-thione towards metal ions of the first transition series, 1705-9
- Axial ligand dissociation of phthalocyaninatoiron(II) adducts. Further evidence for a dissociative mechanism of substitution, 1709-14
- Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20
- HETEROPOLYANION**
- A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- HYDRAZIDE**
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- HYDRAZINE**
- Chemistry of polydentate ligands. Part 3. Ring closures effected by the reaction of β -diketones with 6,6'-dihydrazino- and 6,6'-di-(N-methylhydrazino)-2,2'-bipyridylnickel(II) diperchlorate, 440-6
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridodiruthenium with a series of neutral donor ligands, 1036-9
- Structural studies of substituted hydrazine complexes. Part 2. Crystal and molecular structure of (η -cyclo-octa-1,5-diene)tris(NN-dimethylhydrazine)hydridoruthenium(II) hexafluorophosphate, 1040-2
- Structural studies of substituted hydrazine complexes. Part 3. Crystal and molecular structure of dichlorobis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihydridodiruthenium, an asymmetric triply bridged dimer containing a bidentate bridging NN-dimethylhydrazine ligand, 1043-6
- HYDRAZONATE**
- Electron spin resonance spectra of trigonal-prismatic bis(pentane-2,4-dione benzoylhydrazonato(2-))vanadium(IV) and bis(4-phenylbutane-2,4-dione benzoylhydrazonato(2-))vanadium(IV), 423-6
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- HYDRIDE**
- A molecular-orbital evaluation of skeletal electron-counting procedures, 18-25
- Effects of extra hydrogens on the electronic structures of five- and six-vertexed polyhedral boranes, 25-31
- Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetonitrile complexes of rhodium and iridium, 50-3
- Carbon-13 nuclear magnetic resonance study of osmium complexes of the type $(\text{Os}_3(\text{CO})_{10}\text{H}(\text{X}))$, 196-8
- Preparation of (η -cyclo-octa-1,5-diene)halogenohydrido-bis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cyclo-octa-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
- Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56
- Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Crystal and molecular structure of hydrido(tetrahydroborato)bis(tricyclohexylphosphine)nickel(II), 482-5
- Some binuclear hydrides of platinum, 516-22
- Preparation of uncoordinated hydridoaluminum tetrahydroborate compounds, $\text{Al}(\text{BH}_4)_3 \cdot x\text{H}_x$ ($x = 1$ or 2), and alane (AlH_3) species, 572-7
- The gadolinium-hydrogen system, 601-4
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyltetrahydrotetraosmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-tetrakis(tricarbonyl)osmium(4Os-Os), 673-6
- Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
- Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine)diplatinum complexes: crystal and molecular structure of di- μ -hydrido-bis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
- Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
- Nuclear magnetic resonance studies of the addition of hydrogen halides to trans-cyanohydrido-bis(triethylphosphine)platinum(II) and hydridotris(triethylphosphine)platinum(II) tetraphenylborate 877-9
- Fluorophosphine complexes of ruthenium and osmium. Part 1. Syntheses and stereochemistry of dihydrido-complexes of ruthenium(II) and osmium(II), 885-9
- Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine)

- ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9
- Structural studies of substituted hydrazine complexes. Part 2. Crystal and molecular structure of (η -cyclo-octa-1,5-diene)tris(NN-dimethylhydrazine)hydridoruthenium(II) hexafluorophosphate, 1040-2
- Structural studies of substituted hydrazine complexes. Part 3. Crystal and molecular structure of dichlorobis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihydridoruthenium, an asymmetric triply bridged dimer containing a bidentate bridging NN-dimethylhydrazine ligand, 1043-6
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxy-OP)(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)-C³PO₃(methyl isocyanide)iridium(III), 1119-26
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
- Platinum hydrides containing silyl or germyl ligands. Crystal structure of trans-hydrido-silyl-bis(tricyclohexylphosphine)platinum(II), 1167-70
- Trisium clusters derived from benzylamine and benzyl alcohol: formation of a μ_3 -o-phenylene complex in the conversion of benzyl alcohol into benzene, 1201-6
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarboxylferrates and tricarboxyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304
- The chemistry of polynuclear compounds. Part 31. Synthesis of undecacarbonylhydridotriosmate(1-) and its reaction with octadecacarbonylhexaoxmium to give a carboxylate-bridged anionic enneaoxmium species, 1358-63
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14
- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- Reactions of dodecacarbonyl-triangulo-triruthenium and dodecacarbonyltetrahydridotetraruthenium with mixtures of cyclic polyolefins, 1523-8
- Reactions of methylenecyclopropane with some hydridoplatinum(II) complexes, 1736-9
- Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45
- HYDROBORATE**
Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
- HYDROGEN**
The gadolinium-hydrogen system, 601-4
The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyltetrahydridotetraoxmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-trakis(tricarboxyloxmium)(4Os-Os), 673-6
- HYDROGENATION**
Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
Tetramethylthiophene complexes of rhodium, iridium, palladium, and ruthenium, 857-61
Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15
- HYDROLYSIS**
Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
Structural and mechanistic studies of coordination compounds. Part 20. Preparation and base hydrolysis of some cobalt(III) complexes of quadridentate macrocyclic amines, 216-21
Kinetics of base hydrolysis of cis-aminebromobis(ethylenediamine)cobalt(III) complexes in aqueous solutions at 25°C, 556-60
Structural and mechanistic studies of coordination compounds. Part 21. Base hydrolysis of some trans-tetraaminedichlororuthenium(III) cations, 740-3
Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000
Base hydrolysis of amino-acid esters and amides in the coordination sphere of cobalt(III). Part 3. Hydrolysis of methyl and ethyl 4-aminobutanoate, 1046-51
Analysis of the effects of solvent on the initial and transition states in the kinetics of reaction between tris(1,10-phenanthroline)iron(II) cation and hydroxide ions in methanol- and acetone-water mixtures, 1086-90
Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
Structural and mechanistic studies of coordination compounds. 22. Preparation and ligand-substitution kinetics of trans-dihalogeno- and trans-halogenoisothiocyanato-cobalt(III) complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-tetra-azabicyclo[11.3.1]-heptadeca-1(17),2,11,13,15-pentene, 1180-5
Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- HYDROXYLAMINE**
Sulphur-nitrogen compounds. Part 5. The oxidation of N-aryl-N-(arylsulphonyl)hydroxylamines: preparation of N-aryl-NO-bis(arylsulphonyl)hydroxylamines, 604-7
Kinetic and isotopic studies on the reaction of nitrous acid with cis-chlorobis(ethylenediamine)(hydroxylamine)cobalt(III), 1634-7
- IMINE**
⁵⁷Fe-¹A₁ transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- INDIUM**
Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- IODINE**
Crystal structure of trichlorosulphonium(IV) tetrachloroiodate(III), 1723-5
- ION PAIR**
Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
- ION RADIUS**
Soft-sphere ionic radii for Group 1 and Group 2 metal halides and ammonium halides, 1631-4
- IR**
Photochemistry of carbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarboxylnitrosylmanganese, tricarboxyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarboxyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm⁻¹ region, 262-7
Vibrational spectra of some trichloromethyl- and trifluoromethylmercury(II) compounds, 328-32
Infrared and Raman spectroscopic studies of conformations in liquid and solid triethyl-, diethyl(methyl)- and ethyldimethylphosphines, -phosphines, and -arsines, 388-94
Co-condensation reactions of uranium tetrafluoride and hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40
Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6
Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their

- protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Reactions of strained organosilicon heterocycles with nonacarbonyliron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Molecular vibrations of zirconium(IV) tetrahydroborate, a compound containing triple hydrogen bridges, 710-22
- Preparation and properties of some silyl- and germlyl-halogenoacetylenes and of digermylacetylene, 759-63
- Metal complexes of sulphur ligands. 16. Reaction of trichlorotris(dimethylphenylphosphine)ruthenium and dichlorotris(triphenylphosphine)ruthenium with sodium and ammonium monothiobenzoates: structure of (4-amino-2-imino-4-methylpentane)bis(dimethylphenylphosphine)bis(monothiobenzoato)ruthenium(II), 769-75
- Single-crystal infrared study and assignment for mercury(II) chloride and bromide, 776-82
- Single-crystal Raman and infrared study of aluminium trichloride hexahydrate, 782-8
- Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44
- Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Preparation and vibrational spectra of tetra-*n*-propylammonium carbonyldichloro-organoplatinate(II) salts, and a comparison of their carbon-13 and platinum-195 nuclear magnetic resonance properties with those of organomercury compounds, 872-6
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy 921-5
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-*o*-tolyl phosphite iridium(III) complexes, 926-31
- Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43
- Complexes with sulphur and selenium donor ligands. Part 7. The crystal and molecular structure of bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- Azomethine derivatives. Part 18. Diphenyl-, di-*p*-tolyl-, and di-*tert*-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Coordination bond properties in phthalocyaninatometal(II) complexes. Part 1. Stereochemistry and bond properties in bis(4-methylpyridine)phthalocyaninatometal(II)-4-methylpyridine (1/2) (metal = cobalt or iron), 1018-24
- An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonyl(η -dienyl)isocyanidediiron complexes, 1185-9
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Chromium(II) chemistry. Part 12. Further examples of ferromagnetic chlorochromates(II), 1236-40
- Derivatives of bivalent germanium, tin, and lead. Part 21. Tin(II) formate: a reinvestigation, 1274-8
- Metal complexes of uridine and thymidine, 1294-7
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Acceptor properties of some *o*-phenylenedioxy-derivatives of phosphorus(V) chloride, 1465-71
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- Complexes of osmium(VI) with catechol and substituted catechols, 1501-6
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine) molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
- Complexes with sulphur and selenium donor ligands. Part 8. Some 4-phenylthiosemicarbazone complexes of cobalt(II) and the crystal structure of bis(acetone 4-phenylthiosemicarbazone) cobalt(II) bromide (green form), 1549-54
- Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
- Preparation and physicochemical characterization of anionic uranyl β -ketoenolates, 1618-21
- Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
- Structure and properties of cis-bis(dicyclohexylphosphine) dihalogenonickel(II) complexes, 1671-7
- Complexes of palladium(II) with nucleosides. Preparation and properties of complexes of the type potassium trichloro(nucleoside)palladate(II), 1691-5
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- Versatility of the coordination behaviour of 1-methylpyrimidine-2-thione towards metal ions of the first transition series, 1705-9
- Carbonylhalogeno(*o*-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate *o*-phenylenebis(dimethylarsine), 1726-32
- Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- ### IRIDIUM
- Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetylamine complexes of rhodium and iridium, 50-3
- Preparation of (η -cycloocta-1,5-diene) halogenohydrido-bis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
- The chemistry of carbonyl(phenylethynyl)bis(triphenylphosphine) iridium(I), 381-7
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacetal ligands, 486-95
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-*o*-tolyl phosphite iridium(III) complexes, 926-31
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-*tert*-butylphosphine: crystal structure of (2-di-*tert*-butylphosphino-3-methoxyphenoxy-OP)(2-(2-hydroxy-6-methoxyphenyl)-*tert*-butylphosphino)-2-methylpropanoate(2-)-C¹⁸O²(methyl isocyanide)iridium(III), 1119-26
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of (M(C₅Me₅(*so*)₃)(PF₆)₂) (M = Rh or Ir; *so* = MeCN, Me₂CO, or MeOH) with mono-, di-, and tri-

- olefins, 1305-11
- Structures of binary carbonyls and related compounds. Part 1. A new approach to fluxional behaviour, 1554-68
- Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
- Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5
- ### IRON
- Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium, 31-5
- Crystal and molecular structure and some properties of pyridinium μ -oxobis(trichloroferrate(III))-pyridine, 80-4
- Crystal and molecular structures of (NN'-(2-(2'-pyridyl)ethyl)ethylenebis(salicylideneiminato))iron(II) and -cobalt(II)-ethanol (1/1), 185-91
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7
- Dicarbonyl(η -cyclopentadienyl)iron(II) derivatives of pentaborane(9), 237-44
- Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7
- Preparation and reactions of triphenylphosphine and triphenyl phosphite complexes of (benzylideneacetone)dicarbonyliron(0), 369-73
- Synthesis and molecular structure of bis(μ_3 -but-1-yn-1-yl)undecacarbonyl-quattro-tetrairon (4 Fe-Fe), 419-23
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- Kinetics and mechanism of replacements in pentacyano(ligand)ferrate(II) ions. An attempt to distinguish between the D and I_d mechanisms, 500-2
- Transition-metal carbonyl derivatives of the germanes. Part 6. The methylgermyl iron carbonyl system, 506-11
- ^{57}Fe - ^{14}N transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
- Synthesis and crystal structure of heptacarbonyl- μ_3 -(pent-1-en-1-yl-3-ylidene)-(η -1,2,3-triethylcyclopentadienyl)-triangulo-triiron (3 Fe-Fe): the cleavage of an acetylenic triple bond on a metal-atom cluster, 552-6
- The quenching of excited uranyl ion by d⁶ metallocenes, 569-72
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- He(I) photoelectron spectra of tetracarbonyliron complexes of Group 5 ligands and of olefinic ligands, 695-8
- Transition-metal carbonyl derivatives of the germanes. Part 7. Properties of complexes containing dimethylgermyliron carbonyl groups and their interconversion, 722-6
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborane(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(11), 944-7
- Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6. The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- Coordination bond properties in phthalocyaninatometal(II) complexes. Part 1. Stereochemistry and bond properties in bis(4-methylpyridine)phthalocyaninatometal(II)-4-methylpyridine (1/2) (metal = cobalt or iron), 1018-24
- Analysis of the effects of solvent on the initial and transition states in the kinetics of reaction between tris(1,10-phenanthroline)iron(II) cation and hydroxide ions in methanol- and acetone-water mixtures, 1086-90
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonylbis(η -dienyl)isocyanidediiron complexes, 1185-9
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Reactions of tetracarbonylhydrideferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarbonylferrates and tricarbonyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304
- Reactions of metal carbonyl derivatives. Part 22. The crystal and molecular structures of dicarbonyl(η -cyclopentadienyl)(ethylthio)iron and μ -ethylthio-bis(dicarbonyl(η -cyclopentadienyl)iron) tetrafluoroborate, and a comparison of their molecular parameters, 1379-85
- Heteronuclear cluster systems. Part 12. Synthesis of μ -phenylphosphinediyl-bis(tetracarbonylcobalt) and 1,1,1,2,2,2,3,3,3-nonacarbonyl- μ_3 -phenylphosphinediyl-triangulo-dicobaltiron, 1385-7
- Heteronuclear cluster systems. Part 13. Synthesis of μ -diphenylphosphido-bridged carbonylmetal complexes, and crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3,3-hexacarbonyl-1,3;2,3-bis- μ -diphenylphosphido-triangulo-tricobalt, 1387-92
- Bis(tetrabutylammonium) tetrakis(benzenethiolato- μ_3 -selenidoiron), an iron-selenium cubic cluster compound, 1423-5
- Kinetics and mechanisms of formation, and of reactions, of intermediates in the iron(II)-1,10-phenanthroline-cyanide and related systems, 1447-51
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- Transition-metal carbonyl derivatives of the germanes. Part 9. Reactions of tetracarbonyldi(methylgermyl)iron with some covalent halides, 1569-73
- Solvation effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6
- Kinetics of reaction of imidazole, glycine, and L-histidine with the aquapentacyanoferrate(II) ion, 1610-17
- Reaction of tricarbonyl(2-6- η -hexadienyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82
- Axial ligand dissociation of phthalocyaninatoiron(II) adducts. Further evidence for a dissociative mechanism of substitution, 1709-14
- A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^4 -cyclooctatetraene)(1-6- η^4 -cyclooctatetraene)iron, 1761-6
- ### ISOCYANATE
- Electron-diffraction investigation of the molecular structure of sulphonyl chloride isocyanate, 299-302
- Crystal and molecular structure and magnetic properties of tetrakis((2-diethylaminoethanolato)isocyanatocopper(II)), 1594-8
- ### ISOCYANIDE
- Preparation, structure, and redox properties of isocyanide complexes of molybdenum(0) and tungsten(0), 165-9
- Preparation and structures of ruthenium(III) complexes containing tertiary arsinnes, tertiary phosphines, and isocyanides, 1152-4
- An infrared spectroscopic study of the tautomeric equilibria in solutions of tricarbonylbis(η -dienyl)isocyanidediiron complexes, 1185-9
- Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropanone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
- ### ISOTOPE EFFECT
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- ### KINETICS
- Displacement of organic sulphides by amines in trans-dichlorobis(organic sulphide)palladium(II) complexes, 12-14
- Assignment of the proton-association constants for 3-(3,4-dihydroxyphenyl)alanine (L-dopa), 43-5

- Kinetics and mechanism of oxidation of ascorbic acid by manganese(III) in aqueous acidic perchlorate media, 61-3
- Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10
- A damped nonlinear least-squares computer program (DALFRK) for the evaluation of reaction rate constants, 123-31
- Transient intermediates in the polymerization of tungstate, 133-7
- Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
- Kinetics and mechanism of the reduction of thiocyanato-, isothiocyanato, and azido-pentaamminecobalt(III) by pentaammineaquaruthenium(II) in aqueous solutions, 148-51
- Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino acids, 152-8
- Reactions of platinum(II) complexes. Part 2. Catalysis of the aquation of tetrachloroplatinate(II) ion by trichloro(η -ethylene)platinat(II) (Zeise's anion), 158-9
- Structural and mechanistic studies of coordination compounds. Part 20. Preparation and base hydrolysis of some cobalt(III) complexes of quadridentate macrocyclic amines, 216-21
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7
- Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7
- Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53
- Preparation of (η -cycloocta-1,5-diene)halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- Kinetics and mechanism of replacements in pentacyano(ligand)ferrate(II) ions. An attempt to distinguish between the D and I_d mechanisms, 500-2
- Kinetics and mechanism of the sulphamic acid-nitric acid reaction: evidence for consecutive reactions, 530-4
- Kinetics of base hydrolysis of cis-aminebromobis(ethylenediamine)cobalt(III) complexes in aqueous solutions at 25°C, 556-60
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
- Displacement of chelate ligands from planar four-coordinate complexes. Part 5. Preparation and ligand-substitution reaction of dichloro(ethylenediamine)- and dichloro(propylenediamine)-gold(III) complexes, 728-34
- Structural and mechanistic studies of coordination compounds. Part 21. Base hydrolysis of some trans-tetraaminedichlororuthenium(III) cations, 740-3
- Reaction mechanisms of metal-metal-bonded carbonyls. Part 19. Homolytic fission of bis(tetracarbonyl(triphenylphosphine)manganese)(Mn-Mn) as a path for thermal substitution, 789-93
- Complexes with sulphur and selenium donor ligands. Part 6. Kinetics and mechanism of the reaction between 1,2-bis(diphenylphosphino)ethane and tris(OO'-dimethylphosphorodithioato)cobalt(III), 950-5
- Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6. The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- The reaction between thallium(III) and hydrogen peroxide, 1012-17
- Organosilicon chemistry. Part 21. Reactions of NN'-bistrifluoromethylamino-oxyl and perfluoro(2,4-dimethyl-3-oxa-2,4-diazapentane) with vinylsilanes, and pyrolysis of the resulting adducts, 1024-31
- Base hydrolysis of amino-acid esters and amides in the coordination sphere of cobalt(III). Part 3. Hydrolysis of methyl and ethyl 4-aminobutanoate, 1046-51
- Analysis of the effects of solvent on the initial and transition states in the kinetics of reaction between tris(1,10-phenanthroline)iron(II) cation and hydroxide ions in methanol- and acetone-water mixtures, 1086-90
- Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- Structural and mechanistic studies of coordination compounds. 22. Preparation and ligand-substitution kinetics of trans-dihalogeno- and trans-halogenoisothiocyanato-cobalt(III) complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-tetra-azabicyclo(11.3.1)-heptadeca-1(7),2,11,13,15-pentaene, 1180-5
- A kinetic study of the formation of some unchelated and chelated beryllium(II) complexes in aqueous solutions, 1221-5
- Interaction of vitamin B_{12a} with 8-azaguanine and 6-mercaptopurine: kinetic and thermodynamic characterizations, 1226-32
- Kinetics of the dissociation of decavanadate(6-) in neutral and weakly basic solutions, 1329-33
- Kinetics and mechanisms of formation, and of reactions, of intermediates in the iron(II)-1,10-phenanthroline-cyanide and related systems, 1447-51
- Aspects of the thermal decomposition of ϵ -zinc hydroxide: a kinetic compensation effect, 1484-9
- Dynamic behaviour in solution of some benzo(h)quinoline and 8-methylquinoline complexes of palladium(II), 1497-501
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
- Solvation effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6
- Reactions between copper(II) and 2-mercaptoposuccinic acid in aqueous perchlorate solution, 1606-9
- Kinetics of reaction of imidazole, glycine, and L-histidine with the aquapentacyanoferrate(II) ion, 1610-17
- Kinetic and isotopic studies on the reaction of nitrous acid with cis-chlorobis(ethylenediamine)(hydroxylamine)cobalt(III), 1634-7
- Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
- Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered aniono(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
- Axial ligand dissociation of phthalocyaninatoiron(II) adducts. Further evidence for a dissociative mechanism of substitution, 1709-14
- A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^4 -cyclooctatetraene)(1-6- η^6 -cyclooctatetraene)iron, 1761-6
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide)aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- LACTONE**
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from MoMe(CO)₃(η -C₃H₃) and but-2-yne, 1067-80
- LANTHANIDE**
- Schiff-base complexes of the lanthanoids and actinoids. Part 1. Lanthanoid(III) halide complexes with the unionized form of NN'-ethylenebis(salicylideneimine) and related bases, 36-9
- Preparation and characterization of dithiophosphinato-complexes of yttrium and the lanthanoids, 85-90
- Complexes of lanthanoid salts with the crown ether cis,syn,cis-2,5,8,15,18,21-hexaoxatricyclo(20.4.0.0^{9,14})hexacosane and their paramagnetically shifted nuclear magnetic resonance spectra, 181-4
- A nuclear magnetic resonance investigation of bis(OO'-diethyl dithiophosphato)-complexes of the lanthanoids: separation of

- contact and pseudo-contact contributions to the chemical shifts, 267-72
- Nuclear magnetic resonance studies of lanthanoid complexes. Part 3. Adducts of tris(6,6,7,7,8,8-heptafluoro-2,2-dimethyloctane-3,5-dionato)praseodymium with bidentate amines, 315-19
- LEAD**
- A lead-207 and carbon-13 Fourier-transform nuclear magnetic resonance study of organolead compounds, 960-4
- Equilibria of complex formation between several bivalent metal ions and macrocyclic tri- and penta-amines, 1081-5
- Crystal structure of dilead tritellurate(IV), 1528-32
- LFER**
- Kinetics and mechanism of the reduction of thiocyanato-, isothiocyanato, and azido-pentaamminecobalt(III) by pentaammineaquaruthenium(II) in aqueous solutions, 148-51
- The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms 228-34
- LIQ CRYSTAL**
- The structure of ac-dichloro-b-ethylene-d-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8
- LITHIUM**
- Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodiimide (cyanamide) 1407-11
- LUMINESCENCE QUENCHING**
- The quenching of excited uranyl ion by d^6 metallocenes, 569-72
- MACROCYCLE**
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II): X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10
- Complexes of lanthanoid salts with the crown ether *cis*, *syn*, *cis*-2,5,8,15,18,21-hexaoxatricyclo(20.4.0.0^{9,14})hexacosane and their paramagnetically shifted nuclear magnetic resonance spectra, 181-4
- Structural and mechanistic studies of coordination compounds. Part 20. Preparation and base hydrolysis of some cobalt(III) complexes of quadridentate macrocyclic amines, 216-21
- Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53
- Comparison of the different modes of bonding of the macrocycle in μ -(1,4,8,11-tetrathiacyclotetradecane-S¹S²S³S¹¹)-bis(dichloromercury(II)) and aqua 1,4,8,11-tetrathiacyclotetradecane)mercury(II) perchlorate by X-ray structural analysis, 394-9
- Chemistry of polydentate ligands. Part 3. Ring closures effected by the reaction of β -diketones with 6,6'-dihydrazino- and 6,6'-di-(N-methylhydrazino)-2,2'-bipyridylnickel(II) diperchlorate, 440-6
- A potentially seven-coordinate complex that is only five-coordinate; crystal and molecular structure of di-iodo(6,7,8,9-tetrahydro-16,22-dimethyl-5,10-dithia-15,23,24-triaza-17,21-methenodibenzo(a,i)cyclononadecene-NN'N'')zinc(II), 511-16
- A microcalorimetric study of the macrocyclic effect. Enthalpies of formation of copper(II) and zinc(II) complexes with some tetra-aza macrocyclic ligands in aqueous solution, 577-83
- Ligands for the alkali metals. Part 4. Nuclear magnetic resonance of crown ethers with alkali-metal ions, 611-17
- Reaction of electrogenerated square-planar nickel(I) complexes with alkyl halides, 972-6
- Coordination bond properties in phthalocyaninatometal(II) complexes. Part 1. Stereochemistry and bond properties in bis(4-methylpyridine)phthalocyaninatometal(II)-4-methylpyridine (1/2) (metal = cobalt or iron), 1018-24
- Metal complexes of sexidentate ligands derived from 3-ethoxymethylene-pentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithio)bis(o-phenyleneiminomethylidene)bis(pentane-2,4-dionato)(2-)-nickel(II) and -copper(II), 1057-62
- Equilibria of complex formation between several bivalent metal ions and macrocyclic tri- and penta-amines, 1081-5
- Crystal and molecular structure of trans-diazo(C-meso-5,12-dimethyl-1,4,8,11-tetraazacyclotetradecane)cobalt(III) azide, 1131-4
- Structural and mechanistic studies of coordination compounds. 22. Preparation and ligand-substitution kinetics of trans-dihalogeno- and trans-halogeno-isothiocyanato-cobalt(III) complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-tetra-azabicyclo(11.3.1)-heptadeca-1(17),2,11,13,15-pentaene, 1180-5
- Comparison of the structure and dynamic properties of anion(1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) perchlorate complexes in nitromethane solutions, and the crystal and molecular structure of the chloro complex, 1282-8
- Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- MAGNESIUM**
- Organosubstituted phosphazenes. Part 9. Mass spectra of phenyl-substituted chlorocyclophosphazenes, 173-7
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Neutral, acetate-bridged, binuclear alkyls of rhenium(III), 1063-6
- Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14
- The electronic structure of magnesium dialuminium tetraoxide (spinel) using X-ray emission and X-ray photoelectron spectroscopies, 1785-90
- The electronic structure of magnesium hydroxide (brucite) using X-ray emission, X-ray photoelectron, and Auger spectroscopy, 1791-6
- MAGNETIC CD**
- The magnetic circular-dichroism spectrum of matrix-isolated vanadium hexacarbonyl, 608-11
- MAGNETIC RELAXATION**
- Multinuclear magnetic resonance studies. Part 3. Compounds with phosphorus-oxygen-phosphorus or phosphorus-sulphur-phosphorus bridges, 9-12
- MAGNETISM**
- Magnetic properties of hexakis(pyridine N-oxide)cobalt(II) perchlorate, 160-5
- Low-temperature magnetic studies of a linear trimeric nickel compound: abcikl-hexa-aqua-def:ghi-hexakis(μ -1,2,4-triazole-N¹N²)-trinickel(II) hexanitrate dihydrate, 702-4
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Complexes with sulphur and selenium donor ligands. Part 7. The crystal and molecular structure of bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- Magnetic exchange in some polynuclear bis(azole) dihalogenocopper(II) complexes, 1170-5
- Magnetic susceptibility and optical spectra of the organic-intercalated two-dimensional ferromagnets bis(monomethylammonium)- and bis(monoethylammonium) tetrachlorochromate(II), 1207-12
- Chromium(II) chemistry. Part 12. Further examples of ferromagnetic chlorochromates(II), 1236-40
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine) molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Crystal and molecular structure and magnetic properties of tetrakis(2-diethylaminoethanolato)isocyanatocopper(II), 1594-8

MANGANESE

- Evidence for the formation of the triaquatetracarbonylmanganese(I) cation and related derivatives from pentacarbonylchloromanganese, 4-8
- Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium, 31-5
- Kinetics and mechanism of oxidation of ascorbic acid by manganese(III) in aqueous acidic perchlorate media, 61-3
- Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5
- Crystal and molecular structures of (η -methylcyclopentadienyl)(η -7-exophenylcyclohepta-1,3,5-triene)manganese, 144-7
- Photochemistry of carbonyltrinitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
- Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Cyclometallation reactions. Part 17. Comparative studies of the manganation and palladation of some substituted azobenzenes, 687-94
- Reaction mechanisms of metal-metal-bonded carbonyls. Part 19. Homolytic fission of bis(tetracarbonyl(triphenylphosphine)manganese)(Mn-Mn) as a path for thermal substitution, 789-93
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5
- MASS SPECTRA**
- Organosubstituted phosphazenes. Part 9. Mass spectra of phenyl-substituted chlorocyclophosphazenes, 173-7
- Dicarbonyl(η -cyclopentadienyl)iron(II) derivatives of pentaborane(9), 237-44
- Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Transition-metal carbonyl derivatives of the germanes. Part 7. Properties of complexes containing dimethylgermyliron carbonyl groups and their interconversion, 722-6
- Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63
- Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
- Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43
- Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborate(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(11), 944-7
- Azomethine derivatives. Part 18. Diphenyl-, di-*p*-tolyl-, and di-*tert*-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Trimethylsilyl derivatives for the study of silicate structures. Part 5. Trimethylsilylation of diopside, 1342-9
- Complexes of osmium(VI) with catechol and substituted catechols, 1501-6

- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcobalt, 1752-5

MASS SPECTRAL

- Structure and properties of *cis*-bis(dicyclohexylphosphine)dihalogenonickel(II) complexes, 1671-7

MATRIX

- Photochemistry of carbonyltrinitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
- Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
- Photochemical studies of the alkylammonium molybdates. Part 4. Electron spin resonance study of an irradiated single crystal of hexakis(isopropylammonium) dihydrogen octamolybdate dihydrate, 283-5
- Co-condensation reactions of uranium tetrafluoride and hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40
- The magnetic circular-dichroism spectrum of matrix-isolated vanadium hexacarbonyl, 608-11
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6

MERCURY

- The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms, 228-34
- Structural studies of steric effects in phosphine complexes. Part 3. The synthesis, characterization and molecular structure of diacetato(tris(*tert*-butyl)phosphine)mercury(II), 253-6
- Vibrational spectra of some trichloromethyl- and trifluoromethylmercury(II) compounds, 328-32
- Comparison of the different modes of bonding of the macrocycle in μ -(1,4,8,11-tetrathiacyclotetradecane-S¹S⁴S⁸S¹¹)-bis(dichloromercury(II)) and aqua(1,4,8,11-tetrathiacyclotetradecane)mercury(II) perchlorate by X-ray structural analysis, 394-9
- Reactions of bis(trifluoromethyl)mercury: the synthesis and properties of methyl(trifluoromethyl)-stannanes and -plumbanes, 541-4
- Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6
- Solvation of mercury(II) halides and alkylmercury(II) halides by liquid ammonia: a Raman spectroscopic study, 705-10
- Single-crystal infrared study and assignment for mercury(II) chloride and bromide, 776-82
- Preparation and vibrational spectra of tetra-*n*-propylammonium carbonyldichloro-organoplatinate(II) salts, and a comparison of their carbon-13 and platinum-195 nuclear magnetic resonance properties with those of organomercury compounds, 872-6
- Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5
- Crystal structures of methyl(L-tyrosinato)mercury(II) monohydrate and (L-(2-amino-4-phenylbutanoato)methylmercury(II), 1324-8
- Crystal structure of *exo*-6-chloromercurio-6,7-dihydro-*exo*-7-methoxyaldrin (1,2,3,4,10,10-hexachloro-*exo*-6-chloromercurio-1,4,4a,5,6,7,8,8a-octahydro-*endo*,*exo*-1,4,5,8-dimethano-*exo*-7-methoxynaphthalene), 1573-6
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide) aluminium(III) ion with uni-, bi-, and *ter*-dentate nitrogen-donor ligands in nitromethane solution, 1776-81

MESITYLENE

- Solid-state studies. Part 11. The vibrational spectra of mixed

- crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
- METALLACYCLE**
- Synthesis and crystal structure of 3,3,4-tricyano-2,2-bis(triphenylphosphine)-1-oxa-2-platinacyclobutane, 279-82
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80
- Cobalt metallacycles. Part 5. Synthesis of pyridines from nitriles and acetylenes via cobaltacyclopentadienes, 1278-82
- Crystal and molecular structure of $(\text{Pd}_3(\text{C}_3\text{Ph}(\text{p-MeOC}_6\text{H}_4)_2)_2(\text{acac})_2)$, derived from a triarylcyclopropenium salt and a palladium(0) complex, 1825-30
- The preparation, structures, and reactions of the metallacyclobutenyl complexes $(\text{M}_3(\text{C}_3\text{R}^1\text{R}^2)_2\text{X}_2)$ derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47
- METALLATION**
- Complexes of platinum and palladium with tertiary dimethoxyphenylphosphines: attempts to effect O- or C-metallation, 257-62
- Cyclometallation reactions. Part 17. Comparative studies of the manganate and palladate of some substituted azobenzenes, 687-94
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-o-tolyl phosphite iridium(III) complexes, 926-31
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxo-OP)(2-((2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)-C¹PO²)(methyl isocyanide)iridium(III), 1119-26
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- METALLOACETYLACETONATE**
- Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5
- MICROSCOPY**
- Aspects of the thermal decomposition of ϵ -zinc hydroxide: a kinetic compensation effect, 1484-9
- MO**
- A molecular-orbital evaluation of skeletal electron-counting procedures, 18-25
- Effects of extra hydrogens on the electronic structures of five- and six-vertexed polyhedral boranes, 25-31
- A theoretical investigation of the structure of some small nitrogen-sulphur molecules, 277-9
- Carbonyl(trichlorotris(dimethylphenylphosphine)technetium-ethanol (1/1), the first seven-coordinate complex of technetium; position of this molecule in the C_3 family, 373-80
- Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8
- Molecular and crystal structure of 3,3-bis(triethylphosphine)-1,2-dicarbonyl-3-platinadodecaborane(11), and molecular orbital analysis of the sliq. distortion in carboranellaboranes, 1363-74
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- Photoelectron spectra of metal tetrahydroborates, 1755-61
- The electronic structure of magnesium dialuminium tetraoxide (spinel) using X-ray emission and X-ray photoelectron spectroscopies, 1785-90
- The electronic structure of magnesium hydroxide (brucite) using X-ray emission, X-ray photoelectron, and Auger spectroscopy, 1791-6
- MOESSBAUER**
- Crystal and molecular structure and some properties of pyridinium μ -oxobis(trichloroferrate(III))-pyridine, 80-4
- Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80
- ^{57}Fe - ^{57}Co transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- The gadolinium-hydrogen system, 601-4
- The orientation of the electric-field-gradient tensor from single-crystal Moessbauer measurements, 743-52
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5
- Derivatives of bivalent germanium, tin, and lead. Part 21. Tin(II) formate: a reinvestigation, 1274-8
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- MOLYBDENUM**
- Preparation and characterization of dimeric molybdenum(III)-ethylenediaminetetraacetate complexes, 95-9
- Preparation and properties of new molybdenum-ethylenediaminetetraacetate complexes formed by the oxidation of the molybdenum(III,III) dimer $(\text{Mo}_2(\text{O}_2\text{CMe})(\text{OH})_2(\text{EDTA}))$, 100-4
- Preparation, structure, and redox properties of isocyanide complexes of molybdenum(0) and tungsten(0), 165-9
- Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
- Photochemical studies of the alkylammonium molybdates. Part 4. Electron spin resonance study of an irradiated single crystal of hexakis(isopropylammonium) dihydrogen octamolybdate dihydrate, 283-5
- Structure of (η -allyl)dibicarbonyl(pentane-2,4-dionato)pyridinemolybdenum(II) in the solid and solution states, 291-5
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 7. The fluxional behaviour of bis(cyclopentadienyl)dithiocarbamatomolybdenum complexes, and the application of Forsen-Hoffman spin-saturation method to the nuclear magnetic resonance spectra of a five-spin system, 467-74
- The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9
- The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazono)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- Organosulphur-transition metal chemistry. Part 2. Reactions of

- isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- The standard enthalpies of formation of tris(pentane-2,4-dionato)molybdenum(III) and dioxobis(pentane-2,4-dionato)molybdenum(VI), and the molybdenum-pentane-2,4-dionate bond-enthalpy contributions, 1311-13
- Single-crystal molecular and electronic structure of trichlorooxo(triphenylphosphine sulphide)molybdenum(V), 1350-4
- Inorganic Grignard reagents. Preparations and reactions of (bromobis(tetrahydrofuran)magnesium)bis(η -cyclopentadienyl)hydridomolybdenum, 1510-14
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine)molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Studies in eight-coordination. Part 5. Crystal and molecular structure and electron spin resonance spectra of tetrakis(diethyldithiocarbamate)molybdenum(V) hexamolybdate and chloride, 1582-9
- Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
- Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in arylidiazidotris(dimethyldithiocarbamate)molybdenum, 1654-8
- Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (-)-578-carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino)diphenylphosphine)nitrosylmolybdenum, 1664-70
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- Crystal and molecular structure and electron spin resonance spectrum of trichlorooxobis(triphenylphosphine oxide)molybdenum(V), 1848-54
- NEUTRON SCATTERING**
- Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy 921-5
- NICKEL**
- Resonance-Raman spectra of copper(II) and nickel(II) diethyldithiocarbamates, 53-6
- Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II): X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- Magnetic properties of hexakis(pyridine N-oxide)cobalt(II) perchlorate, 160-5
- Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80
- Standard enthalpies of formation of tris(bis(pentane-2,4-dionato)nickel(II)) and bis(2,2,6,6-tetramethylheptane-3,5-dionato)nickel(II) and an estimation of nickel-oxygen bond energies, 399-402
- Chemistry of polydentate ligands. Part 3. Ring closures effected by the reaction of β -diketones with 6,6'-dihydrazino- and 6,6'-di-(N-methylhydrazino)-2,2'-bipyridylnickel(II) diperchlorate, 440-6
- Crystal and molecular structure of hydrido(tetrahydroborato)bis(tricyclohexylphosphine)nickel(II), 482-5
- $^5\text{T}_2-1\text{A}_1$ transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- Low-temperature magnetic studies of a linear trimeric nickel compound: abcdk-hexa-aqua-def:ghi-hexakis(μ -1,2,4-triazole- N^1N^2)-trinickel(II) hexanitrate dihydrate, 702-4
- A classical polarizability treatment for planar bis(2-(R)-1,2,2-trimethylpropyliminomethyl)naphtholato(1-)-NO)nickel(II), 822-6
- Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44
- Superexchange in linear-chain 2,5-dimethylpyrazinebis(pentane-2,4-dionato)-cobalt(II) and -nickel(II) complexes, 868-71
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Effect of mixed-ligand complex formation on the ionization of the pyrrole hydrogens of histamine and histidine, 964-8
- Reaction of electrogenerated square-planar nickel(I) complexes with alkyl halides, 972-6
- Metal complexes of sexidentate ligands derived from 3-ethoxymethylene-pentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithiobis(o-phenyleneimino)methylidyne)bis(pentane-2,4-dionato)(2-)-nickel(II) and -copper(II), 1057-62
- Empirical force-field calculations of strain-energy contributions to the thermodynamics of complex formation. Part 1. The difference in stability between complexes containing five- and six-membered chelate rings, 1438-44
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- Spectroscopy and reactions of copper(II), nickel(II), and cobalt(III) compounds in molten nitrates, 1589-93
- Structure and properties of cis-bis(dicyclohexylphosphine)dihalogenonickel(II) complexes, 1671-7
- Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered anion(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
- NIOBIUM**
- Crystal structures of octacaesium and octarubidium dicosaniobates 968-72
- NITRIDE**
- Structural studies of nitrido-complexes: X-ray crystal structure of tetraphenylarsonium pentakis(isothiocyanato)nitridorhenate(VI), 844-8
- NITROGEN**
- Organosubstituted phosphazenes. Part 9. Mass spectra of phenyl-substituted chlorocyclophosphazenes, 173-7
- Photochemistry of carbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
- Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
- The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms 228-34
- A theoretical investigation of the structure of some small nitrogen-sulphur molecules, 277-9
- Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Kinetics and mechanism of the sulphamic acid-nitric acid reaction: evidence for consecutive reactions, 530-4
- Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
- Phosphorus-nitrogen-phosphorus spin coupling in the nuclear magnetic resonance spectra of some cyclodiphosph(III)azanes, 634-8
- Crystal and molecular structure of NN-di-isopropyl-P-phenylphosphonamidic chloride, $\text{PPh}(\text{Cl})(\text{NPr}_2)_2\text{O}$, 647-50
- Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- Conformational effects on PNCH, PNC, and PNCSi spin coupling in tervalent phosphorus-nitrogen compounds, 764-9
- Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy 921-5
- Azomethine derivatives. Part 18. Diphenyl-, di-p-tolyl-, and di-tert-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Structural studies on biguanide and related species. Correlation of

- protonation energy with molecular structure, 989-96
 Crystal structure of 2,trans-4,cis-6,trans-8-tetrachloro-2,4,6,8-tetrakis(dimethylamino)cyclotetraphosphazene, 1094-8
 Crystal structure of compounds with (N-P)_n rings. Part 12. Decafluorocyclopentaphosphazene, 1425-30
 Kinetic and isotopic studies on the reaction of nitrous acid with *cis*-chlorobis(ethylenediamine)(hydroxylamine)cobalt(III), 1634-7
 Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
 Dinitrogen trioxide. Part 14. Adduct formation between dinitrogen trioxide and aromatic donors, 1721-3
 Reactions of silane with zeolitic water, 1746-52
 Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- NITROSYL**
 Organometallic nitrosyl chemistry. Part 3. Some aspects of the chemistry of bis(η -cyclopentadienyl)dinitrosylchromium), 31-5
 Photochemistry of carbonyl(trinitrosyl)manganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
 Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
 The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 7. The fluxional behaviour of bis(cyclopentadienyl)dithiocarbamatomolybdenum complexes, and the application of Forsen-Hoffman spin-saturation method to the nuclear magnetic resonance spectra of a five-spin system, 467-74
 The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9
 The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2
 Nitrosyl complexes of rhenium. Part 3. Crystal and molecular structure of tetraethylammonium tetrachloronitrosyl(pyridine)rheneate(1-), 798-801
 Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium-, osmium and -nickel complexes, 837-44
 Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-*tert*-butylphosphine: crystal structure of (2-di-*tert*-butylphosphino-3-methoxyphenoxy-OP)(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)-C(PO₂)(methyl isocyanide)iridium(III), 1119-26
 Studies on transition metal cyano complexes. Part 2. Unsubstituted cyanorhenates, (Re(CN)₅)ⁿ⁻, and cyanorhenates with thio-, seleno-, and nitrosyl ligands, 1411-17
 Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
 Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (-)- γ -carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino)diphenylphosphine)nitrosylmolybdenum, 1664-70
- NMR**
 Multinuclear magnetic resonance studies. Part 3. Compounds with phosphorus-oxygen-phosphorus or phosphorus-sulphur-phosphorus bridges, 9-12
 Preparation and structure of 1,4-dichloro-1,1,3,3-tetraphenylcatena-di(boraphosphane), BH₂Cl.PPh₂.PPh₂.Cl, 40-3
 Complexes of lanthanoid salts with the crown ether *cis*,*syn*,*cis*-2,5,8,15,18,21-hexaoxatricyclo(20.4.0.0^{9,14})hexacosane and their paramagnetically shifted nuclear magnetic resonance spectra, 181-4
 Carbon-13 nuclear magnetic resonance study of osmium complexes of the type (Os₃(CO)₁₀H(X)), 196-8
 Hydrogen-1 nuclear magnetic resonance evidence for trans addition in oxythallation of acyclic olefins, 234-7
 Dicarboxyl(η -cyclopentadienyl)iron(II) derivatives of pentaborane(9), 237-44
 A nuclear magnetic resonance investigation of bis(OO'-diethyl dithiophosphato)-complexes of the lanthanoids: separation of contact and pseudo-contact contributions to the chemical shifts, 267-72
 Monobridged binuclear platinum complexes. Part 1. Some phosphido-bridged diplatinum complexes of triethylphosphine, 272-6
 Carbaborane derivatives of the late- and post-transition elements. Part 1. Preparation and X-ray crystal structure of 3-diethylthiocarbamate-1,2-dicarba-3-auradodecaborane(11), 303-9
 Nuclear magnetic resonance studies of lanthanoid complexes. Part 3. Adducts of tris(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctane-3,5-dionato)praseodymium with bidentate amines, 315-19
 Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
 Hydrocarbon complexes of iron, ruthenium, and osmium. 11. Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3:6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
 The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 7. The fluxional behaviour of bis(cyclopentadienyl)dithiocarbamatomolybdenum complexes, and the application of Forsen-Hoffman spin-saturation method to the nuclear magnetic resonance spectra of a five-spin system, 467-74
 Protonation of the decavanadate(6-) ion: a vanadium-51 nuclear magnetic resonance study, 503-6
 Some binuclear hydrides of platinum, 516-22
 Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron)(Fe-Fe), 534-40
 Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6
 Preparation of uncoordinated hydridoaluminium tetrahydroborate compounds, Al(BH₄)_{3-x}H_x (x = 1 or 2), and alane (AlH₃) species, 572-7
 Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
 Sulphur-nitrogen compounds. Part 5. The oxidation of N-aryl-N-(arylsulphonyl)hydroxylamines: preparation of N-aryl-NO-bis(arylsulphonyl)hydroxylamines, 604-7
 Ligands for the alkali metals. Part 4. Nuclear magnetic resonance of crown ethers with alkali-metal ions, 611-17
 Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
 Phosphorus-nitrogen-phosphorus spin coupling in the nuclear magnetic resonance spectra of some cyclodiphosph(III)azanes, 634-8
 Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
 Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
 Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63
 Conformational effects on PNCH, PNC, and PNCi spin coupling in trivalent phosphorus-nitrogen compounds, 764-9
 Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine)diplatinum complexes: crystal and molecular structure of di- μ -hydridobis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
 Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
 Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis(carbene)ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
 Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-

- carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Tetramethylthiophene complexes of rhodium, iridium, palladium, and ruthenium, 857-61
- Preparation and vibrational spectra of tetra-*n*-propylammonium carbonyldichloro-organoplatinum(II) salts, and a comparison of their carbon-13 and platinum-195 nuclear magnetic resonance properties with those of organomercury compounds, 872-6
- Nuclear magnetic resonance studies of the addition of hydrogen halides to trans-cyanohydridobis(triethylphosphine)platinum(II) and hydridotris(triethylphosphine)platinum(II) tetraphenylborate, 877-9
- Fluorophosphine complexes of ruthenium and osmium. Part 1. Syntheses and stereochemistry of dihydrido-complexes of ruthenium(II) and osmium(II), 885-9
- Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
- Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
- Fluorophosphine complexes of ruthenium and osmium. Part 4. Homobinuclear trichloro-bridged complexes of ruthenium(II), 901-9
- Trichloro-bridged heterobimetallic phosphine complexes containing ruthenium(II) and rhodium(III), 909-12
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-*o*-tolyl phosphite iridium(III) complexes, 926-31
- Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43
- Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborate(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(11), 944-7
- A lead-207 and carbon-13 Fourier-transform nuclear magnetic resonance study of organolead compounds, 960-4
- Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5
- Azomethine derivatives. Part 18. Diphenyl-, di-*p*-tolyl-, and di-*tert*-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52
- Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Comparison of the structure and dynamic properties of anion(1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) perchlorate complexes in nitromethane solutions, and the crystal and molecular structure of the chloro complex, 1282-8
- Use of aryltin compounds in the preparation of diaryl- and diaroyl-di- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- Acceptor properties of tetrachloro(phenyl)phosphorane and of the trichloro(phenyl)phosphonium ion, 1318-23
- Crystal structures of methyl(L-tyrosinato)mercury(II) monohydrate and L-(2-amino-4-phenylbutanoato)methylmercury(II), 1324-8
- The structure of ac-dichloro-b-ethylene-d-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8
- The chemistry of polynuclear compounds. Part 31. Synthesis of undecacarbonylhydridotrisosmate(1-) and its reaction with octadecacarbonylhexaosmium to give a carboxylate-bridged anionic enneaosmium species, 1358-63
- Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di- μ -arylthio-bis(η -cyclopentadienyl)rhodium, 1375-9
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Reactions of some phosphorus(V) halides and halide oxides with strongly acidic solvents, 1455-60
- Acceptor properties of some *o*-phenylenedioxy-derivatives of phosphorus(V) chloride, 1465-71
- Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropanone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl-N)palladium(II) perchlorate, 1490-6
- Dynamic behaviour in solution of some benzo(h)quinoline and 8-methylquinoline complexes of palladium(II), 1497-501
- Complexes of osmium(VI) with catechol and substituted catechols, 1501-6
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
- Transition-metal carbonyl derivatives of the germanes. Part 9. Reactions of tetracarbonyldi(methylgermyl)iron with some covalent halides, 1569-73
- Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
- Preparation and physicochemical characterization of anionic uranyl β -ketoenolates, 1618-21
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacetal ligands, 1647-53
- Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in arylidiazeneditris(dimethyldithiocarbamate)molybdenum, 1654-8
- Dealkylation of chelating ethers by reaction with WCl₄Y (Y = O, S, Se, or NC₂Cl₂), 1658-61
- Structure and properties of cis-bis(dicyclohexylphosphine)dihalogenonickel(II) complexes, 1671-7
- Reaction of tricarbonyl(2- η -hexadecenyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82
- Complexes of palladium(II) with nucleosides. Preparation and properties of complexes of the type potassium trichloro(nucleoside)palladate(II), 1691-5
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- Carbonylhalogeno(*o*-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate *o*-phenylenebis(dimethylarsine), 1726-32
- Some cyclopropylplatinum complexes, 1732-5
- Reactions of methylenecyclopropane with some hydridoplatinum(II) complexes, 1736-9
- Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45
- Transition-metal carbonyl derivatives of the germanes. Part 10. Tetracarbonyldigermanylcoalt, 1752-5
- A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^6 -cyclooctatetraene)(1-6- η^6 -cyclooctatetraene)iron, 1761-6
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide)aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- Trans-influence of anionic, neutral, and bridging ligands on the nuclear magnetic resonance spectra of methyl- and fluorobenzyl-bis(dimethylglyoximate)rhodium(III) complexes. Some observations on bridge formation, 1807-13
- Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20

687-94

NQR

- Acceptor properties of tetrachloro(phenyl)phosphorane and of the trichloro(phenyl)phosphonium ion, 1318-23
Acceptor properties of some *o*-phenylenedioxy-derivatives of phosphorus(V) chloride, 1465-71

NTA

- Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18

NUCLEAR FUSION

- Solutions of lithium salts in liquid lithium: preparation and X-ray crystal structure of the dilithium salt of carbodiimide (cyanamide), 1407-11

NUCLEOPHILIC

- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12

NUCLEOSIDE

- Metal complexes of uridine and thymidine, 1294-7
Complexes of palladium(II) with nucleosides. Preparation and properties of complexes of the type potassium trichloro(nucleoside)palladate(II), 1691-5

OLEFIN

- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of $(M(C_5Me_5(sol)_3)(PF_6)_2$ ($M = Rh$ or Ir ; $sol = MeCN, Me_2CO$, or $MeOH$) with mono-, di-, and tri-olefins, 1305-11
Reactions of dodecacarbonyl-triangulo-triruthenium and dodecacarbonyltetrahydrotetrairuthenium with mixtures of cyclic polyolefins, 1523-8

OLEUM

- Reactions of some phosphorus(V) halides and halide oxides with strongly acidic solvents, 1455-60

ORD

- Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino acids, 152-8

OSMIUM

- Carbon-13 nuclear magnetic resonance study of osmium complexes of the type $(Os_3(CO)_{10}H(X))$, 196-8
The quenching of excited uranyl ion by d^6 metallocenes, 569-72
The chemistry of polynuclear compounds. Part 30. Some reactions of dodecacarbonyltetrahydrotetraosmium: the molecular and crystal structure of trihydrido- μ_2 -iodo-cyclo-tetrakis(tricarbonylosmium)(4Os-Os), 673-6
Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium-, -osmium and -nickel complexes, 837-44
Fluorophosphine complexes of ruthenium and osmium. Part 1. Syntheses and stereochemistry of dihydrido-complexes of ruthenium(II) and osmium(II), 885-9
Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
Triosmium clusters derived from benzylamine and benzyl alcohol: formation of a μ_3 -*o*-phenylene complex in the conversion of benzyl alcohol into benzene, 1201-6
The chemistry of polynuclear compounds. Part 31. Synthesis of undecacarbonylhydridotriosmate(1-) and its reaction with octadecacarbonylhexaosmium to give a carboxylate-bridged anionic enneaosmium species, 1358-63
Complexes of osmium(VI) with catechol and substituted catechols, 1501-6
Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
Carbonylhalogeno(*o*-phenylenebis(dimethylarsine))osmium complexes, including those containing unidentate *o*-phenylenebis(dimethylarsine), 1726-32

OXADIPHOSPHANE

- Multinuclear magnetic resonance studies. Part 3. Compounds with phosphorus-oxygen-phosphorus or phosphorus-sulphur-phosphorus bridges, 9-12

OXIDATIVE ADDN

- Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8

OXIDN

- Kinetics and mechanism of oxidation of ascorbic acid by manganese(III) in aqueous acidic perchlorate media, 61-3
Preparation and properties of new molybdenum-ethylenediaminetetraacetate-complexes formed by the oxidation of the molybdenum(III,III) dimer $(Mo_2(O_2CMe)(OH)_2(EDTA))$, 100-4
Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
Preparation of (η -cycloocta-1,5-diene) halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56
Sulphur-nitrogen compounds. Part 5. The oxidation of N-aryl-N-(arylsulphonyl)hydroxylamines: preparation of N-aryl-NO-bis(arylsulphonyl)hydroxylamines, 604-7
Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
Kinetics of oxidation of dichlorobis(substituted pyridine) platinum(II) and of reduction of tetrachlorobis(substituted pyridine)platinum(IV) complexes, 699-702
Characterization of degradation products in the oxidation of the dodecahydro-7,8-dicarba-nido-undecaborate(1-) ion: a new synthesis of 4,5-dicarba-nido-nonaborane(1), 944-7
Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine) trisothiocyanatatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarbonylferrates and tricarbonyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304
Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di- μ -aryltio-bis(η -cyclopentadienyl)rhodium), 1375-9
Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
OXIDN ADDN
Triosmium clusters derived from benzylamine and benzyl alcohol: formation of a μ_3 -*o*-phenylene complex in the conversion of benzyl alcohol into benzene, 1201-6
Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
Binuclear diaryltriazenido- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
Some cyclopropylplatinum complexes, 1732-5
OXIMATE
Nitrogen derivatives of iron carbonyls. Part 5. New routes in the mechanism of reaction of dodecacarbonyl-triangulo-triiron with nitroalkanes, and X-ray analysis of μ -(acetone oximate(1-)-NO)- μ -isopropylamido-bis(tricarbonyliron) (Fe-Fe), 534-40
Trans-influence of anionic, neutral, and bridging ligands on the

- nuclear magnetic resonance spectra of methyl- and fluorobenzyl-bis(dimethylglyoximate)rhodium(III) complexes. Some observations on bridge formation, 1807-13
- Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20
- OXYGEN**
- Coordinative tin-oxygen interactions in dinitratodiphenyl(triphenylphosphine oxide)tin(IV), 131-3
- Crystal and molecular structure of (dioxigen)(NN'-(2-(2'-pyridyl)ethyl)ethylenebis(salicylideneiminato))cobalt-acetonitrile (1/1), 191-6
- Some oxygen-donor complexes of cyclopentadienyluranium(IV) halides, 295-8
- A structural theory for nonstoichiometry. Part 4. Defect fluorite-type structures: vacancy superstructures in ordered calcium oxide-hafnium dioxide ternary oxides, 320-8
- Standard enthalpies of formation of tris(bis(pentane-2,4-dionato)nickel(II)) and bis(2,2,6,6-tetramethylheptane-3,5-dionato)nickel(II) and an estimation of nickel-oxygen bond energies, 399-402
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- Reactions of tellurium oxides with alkali-metal oxides and hydroxides, 948-50
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxy-OP(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanato(2-)-ClPO₂)(methyl isocyanide)iridium(III), 1119-26
- Dinitrogen trioxide. Part 14. Adduct formation between dinitrogen trioxide and aromatic donors, 1721-3
- Reactions of silane with zeolitic water, 1746-52
- OXYL**
- Organosilicon chemistry. Part 21. Reactions of NN'-bis(trifluoromethylamino)-oxyl and perfluoro(2,4-dimethyl-3-oxa-2,4-diazapentane) with vinylsilanes, and pyrolysis of the resulting adducts, 1024-31
- PALLADIUM**
- Displacement of organic sulphides by amines in trans-dichlorobis(organic sulphide)palladium(II) complexes, 12-14
- Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80
- Complexes of platinum and palladium with tertiary dimethoxyphenylphosphines: attempts to effect O- or C-metallation, 257-62
- Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14
- Cyclometallation reactions. Part 17. Comparative studies of the manganation and palladation of some substituted azobenzenes, 687-94
- Mixed-ligand complexes of palladium(II). Part 3. Diaqua(ethylenediamine)palladium(II) complexes of L-amino-acids, 726-8
- Displacement of chelate ligands from planar four-coordinate complexes. Part 5. Preparation and ligand-substitution reaction of dichloro(ethylenediamine)- and dichloro(propylenediamine)-gold(III) complexes, 728-34
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Metal complexes of sulphur ligands. Part 17. Reaction of palladium(II) and platinum(II) monoethoxybenzoates with various Lewis bases and further studies on complexes containing related ligands, 1195-200
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl-N)palladium(II) perchlorate, 1490-6
- Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
- Electronic and resonance-Raman spectra of mixed-valence ammine complexes of palladium and platinum, 1622-7
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- Complexes of palladium(II) with nucleosides. Preparation and properties of complexes of the type potassium trichloro(nucleoside)palladate(II), 1691-5
- Crystal and molecular structure of (Pd₃(C₃Ph(p-MeOC₆H₄)₂)₂(acac)₂), derived from a triarylcyclopropenium salt and a palladium(0) complex, 1825-30
- The preparation, structures, and reactions of the metallocyclobutenyl complexes (M₃(C₃R¹R²)₂X₂) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- PENICILLAMINE**
- Gold complexes of L-cysteine and D-penicillamine, 199-201
- PENTALENE**
- Hydrocarbon complexes of iron, ruthenium, and osmium. 11. Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3,6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
- Crystal and molecular structure of μ -pentalenebis(dicarbonyl(trimethylgermyl)ruthenium), 412-16
- PEROXIDE**
- The reaction between thallium(III) and hydrogen peroxide, 1012-17
- PHASE DIAGRAM**
- Dinitrogen trioxide. Part 14. Adduct formation between dinitrogen trioxide and aromatic donors, 1721-3
- PHOSPHATHIANE**
- Multinuclear magnetic resonance studies. Part 3. Compounds with phosphorus-oxygen-phosphorus or phosphorus-sulphur-phosphorus bridges, 9-12
- PHOSPHAZANE**
- Phosphorus-nitrogen-phosphorus spin coupling in the nuclear magnetic resonance spectra of some cyclodiphosph(III)azanes, 634-8
- PHOSPHAZENE**
- Crystal structure of 2,trans-4,cis-6,trans-8-tetrachloro-2,4,6,8-tetrakis(dimethylamino)cyclotetraphosphazene, 1094-8
- Crystal structure of compounds with (N-P)_n rings. Part 12. Decafluorocyclopentaphosphazene, 1425-30
- PHOSPHINE**
- Unsaturated σ -hydrocarbyl transition-metal complexes. Part 4. Crystal and molecular structure of trans-chlorobis(diethylphenylphosphine)(phenylethynyl)platinum(II) and comments on the relative trans influence of various carbon ligands, 46-50
- Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetamide complexes of rhodium and iridium, 50-3
- Ruthenium complexes containing Group 5B donor ligands. Part 5. Synthesis and crystal and molecular structure of acetone(carbonyl)chloro(trichlorostannio)bis(triphenylphosphine)ruthenium(II)-acetone (1/1), 76-9
- Schiff-base complexes of ruthenium(II), 110-15
- Coordinative tin-oxygen interactions in dinitratodiphenyl(triphenylphosphine oxide)tin(IV), 131-3
- Electrolysis of borane anions at reactive metal anodes: a convenient route to metallaboranes, 141-4
- Preparation, structure, and redox properties of isocyanide complexes of molybdenum(0) and tungsten(0), 165-9
- Gold complexes of L-cysteine and D-penicillamine, 199-201
- Structural studies of steric effects in phosphine complexes. Part 3. The synthesis, characterization and molecular structure of diacetato(tris(tert-butyl)phosphine)mercury(II), 253-6
- Complexes of platinum and palladium with tertiary dimethoxyphenylphosphines: attempts to effect O- or C-metallation, 257-62
- Monobridged binuclear platinum complexes. Part 1. Some phosphido-bridged diplatinum complexes of triethylphosphine, 272-6
- Synthesis and crystal structure of 3,3,4-tricyano-2,2-bis(triphenylphosphine)-1-oxa-2-platinacyclobutane, 279-82
- Preparation of (η -cycloocta-1,5-diene)

- halogenohydridobis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7
- Carbene complexes. Part 13. The synthesis and characterization of secondary carbene complexes of vanadium(I), chromium(0), molybdenum(0), tungsten(0), manganese(I), rhenium(I), iron(0), ruthenium(II), cobalt(I), iridium(III), and platinum(IV), and hydridorhodium(III), 348-56
- Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
- Preparation and reactions of triphenylphosphine and triphenyl phosphite complexes of (benzylideneacetone)dicarbonyliron(0), 369-73
- Carbonyltrichlorotris(dimethylphenylphosphine)technetium-ethanol (I/1), the first seven-coordinate complex of technetium; position of this molecule in the C_{3v} family, 373-80
- The chemistry of carbonyl(phenylethynyl)bis(triphenylphosphine)iridium(I), 381-7
- Infrared and Raman spectroscopic studies of conformations in liquid and solid triethyl-, diethyl(methyl)- and ethyldimethylamines, -phosphines, and -arsines, 388-94
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 8. Carboxylato- and β -diketonato-complexes, their reactions with water, hydrogen sulphide, and alcohols, and the treatment of bis(cyclopentadienyl)iodonitrosylmolybdenum with some acids, 474-9
- Crystal and molecular structure of hydrido(tetrahydroborato)bis(tricyclohexylphosphine)nickel(II), 482-5
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- Some binuclear hydrides of platinum, 516-22
- Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
- Trimethylphosphine oxide complexes of thorium and uranium tetranitrates: crystal structures of ten- and twelve-coordinate complex ions, bis(trinitratotetrakis(trimethylphosphine oxide)thorium(IV)) hexanitratothorane(IV) and tetraphenylphosphonium pentanitrato bis(trimethylphosphine oxide)thorane(IV), 638-46
- Crystal and molecular structure of dichlorodioxobis(triphenylphosphine oxide)uranium(VI), 677-80
- Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
- Conformational effects on PNCH, PNC, and PNSi spin coupling in tervalent phosphorus-nitrogen compounds, 764-9
- Metal complexes of sulphur ligands. 16. Reaction of trichlorotris(dimethylphenylphosphine)ruthenium and dichlorotris(trimethylphosphine)ruthenium with sodium and ammonium monothiobenzoates; structure of (4-amino-2-imino-4-methylpentane)bis(dimethylphenylphosphine) bis(monothiobenzoato)ruthenium(II), 769-75
- Reaction mechanisms of metal-metal-bonded carbonyls. Part 19. Homolytic fission of bis(tetracarbonyl(triphenylphosphine)manganese)(Mn-Mn) as a path for thermal substitution, 789-93
- Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine)diplatinum complexes: crystal and molecular structure of di- μ -hydridobis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenenitrosylruthenium, -osmium and -nickel complexes, 837-44
- Nuclear magnetic resonance studies of the addition of hydrogen halides to trans-cyanohydridobis(triethylphosphine)platinum(II) and hydridotris(triethylphosphine)platinum(II) tetraphenylborate, 877-9
- Fluorophosphine complexes of ruthenium and osmium. Part 1. Syntheses and stereochemistry of dihydrido-complexes of ruthenium(II) and osmium(II), 885-9
- Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
- Fluorophosphine complexes of ruthenium and osmium. Part 4. Homobinuclear trichloro-bridged complexes of ruthenium(II), 901-9
- Trichloro-bridged heterobimetallic phosphine complexes containing ruthenium(II) and rhodium(III), 909-12
- Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15
- Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-o-tolyl phosphite iridium(III) complexes, 926-31
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Complexes with sulphur and selenium donor ligands. Part 6. Kinetics and mechanism of the reaction between 1,2-bis(diphenylphosphino)ethane and tris(OO'-dimethyl phosphorodithioato)cobalt(III), 950-5
- Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5
- Azomethine derivatives. Part 18. Diphenyl-, di-p-tolyl-, and di-tert-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine) ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from MoMe(CO)₃(η -C₃H₃) and but-2-yne, 1067-80
- Thermochemistry of dichlorobis(triphenylphosphine oxide)-zinc(II) -cadmium(II), and -mercury(II), 1102-4
- Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxy-OP)(2-(2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropanoate(2-)-C¹PO²(methyl isocyanide)iridium(III), 1119-26
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5
- Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52
- Preparation and structures of ruthenium(III) complexes containing tertiary arsines, tertiary phosphines, and isocyanides, 1152-4
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Platinum hydrides containing silyl or germyl ligands. Crystal structure of trans-hydridosilyl-bis(tricyclohexylphosphine)platinum(II), 1167-70
- Crystal and molecular structure of di- μ -bromo- μ -tetraphenyldiphosphane-bis(tricarbonylrhenium(I)), 1189-95
- Metal complexes of sulphur ligands. Part 17. Reaction of palladium(II) and platinum(II) monothiobenzoates with various Lewis bases and further studies on complexes containing related

- ligands, 1195-200
- Oxidative addition of carboxylic acids to trans-carbonylhalogenobis(tertiary phosphine)iridium(I) complexes, 1213-20
- Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine)trisothiocyanatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- Cobalt metallacycles. Part 5. Synthesis of pyridines from nitriles and acetylenes via cobaltacyclopentadienes, 1278-82
- Use of aryltin compounds in the preparation of diaryl- and diaryldi- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- Crystal and molecular structure of di- μ -trimethylsilylmethyl-bis(trimethylphosphine)(trimethylsilylmethyl)chromium(II) (4Cr-Cr), 1314-18
- Synthesis and dynamic behaviour of bis(ethylene)(tertiary phosphine)platinum complexes, 1337-42
- Single-crystal molecular and electronic structure of trichlorooxo(triphenylphosphine sulphide)molybdenum(V), 1350-4
- Molecular and crystal structure of 3,3-bis(triethylphosphine)-1,2-dicarba-3-platinadodecaborane(11), and molecular orbital analysis of the slip distortion in carbametalboranes, 1363-74
- Heteronuclear cluster systems. Part 12. Synthesis of μ -phenylphosphinediyl-bis(tetracarbonylcobalt) and 1,1,1,2,2,2,3,3,3-nonacarbonyl- μ_3 -phenylphosphinediyl-triangular-dicobaltiron 1385-7
- Heteronuclear cluster systems. Part 13. Synthesis of μ -diphenylphosphido-bridged carbonylmetal complexes, and crystal structure of 1,2- μ -carbonyl-1,1,2,2,3,3-hexacarbonyl-1,3; 2,3-bis- μ -diphenylphosphido-triangular-tricobalt, 1387-92
- Addition reactions on coordinated olefinic ligands. Part 8. Platinum(II) complexes of 1,1-dimethylallene and their reaction with amines. Molecular structure of the zwitterionic derivative dichloro(1-(NN-diethylammoniomethyl)-2-methylprop-1-enyl)(triphenylphosphine)platinum(II), 1392-7
- Complexes of 2-chloroethoxybis(trifluoromethyl)phosphine with carbonyls of manganese, iron, and cobalt, 1452-4
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- 1,2-Bis(arylimino)propylpalladium complexes as N-donor chelate ligands towards metals of the first transition series, 1478-84
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- Binuclear diaryltriazene- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine)molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
- Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
- Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- Absolute configurations of organometallic compounds. Part 6. The crystal structure and absolute configuration of (-)-578-carbonyl(η -cyclopentadienyl)((S)-methyl(1-phenylethyl)amino)diphenylphosphine)nitrosylmolybdenum, 1664-70
- Structure and properties of cis-bis(dicyclohexylphosphine)dihalogenonickel(II) complexes, 1671-7
- Reaction of tricarbonyl(2-6- η -hexadienyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82
- Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered anion(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
- Complexes of platinum metals with crown ethers containing tertiary phosphine-substituted benzo groups, 1696-705
- Some cyclopropylplatinum complexes, 1732-5
- Reactions of methylenecyclopropane with some hydrido-platinum(II) complexes, 1736-9
- Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5
- The preparation, structures, and reactions of the metallacyclobutenyl complexes ($M_3(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47
- Crystal and molecular structure and electron spin resonance spectrum of trichlorooxobis(triphenylphosphine oxide)molybdenum(V), 1848-54
- PHOSPHINODITHIOATE**
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- PHOSPHORANE**
- Acceptor properties of tetrachloro(phenyl)phosphorane and of the trichloro(phenyl)phosphonium ion, 1318-23
- PHOSPHOROUS**
- Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
- PHOSPHORUS**
- Preparation and structure of 1,4-dichloro-1,1,3,3-tetraphenylcatena-di(boraphosphane), $BH_2Cl.PPh_2.BH_2.PPh_2Cl$, 40-3
- Organosubstituted phosphazenes. Part 9. Mass spectra of phenyl-substituted chlorocyclophosphazenes, 173-7
- A nuclear magnetic resonance investigation of bis(OO'-diethyl dithiophosphato)-complexes of the lanthanoids: separation of contact and pseudo-contact contributions to the chemical shifts, 267-72
- Some oxygen-donor complexes of cyclopentadienyluranium(IV) halides, 295-8
- The crystal structure of tin(II) bis(dihydrogenphosphate), 566-9
- Phosphorus-nitrogen-phosphorus spin coupling in the nuclear magnetic resonance spectra of some cyclodiphosph(III)azanes, 634-8
- Crystal and molecular structure of NN-di-isopropyl-P-phenylphosphonamidic chloride, $PPh(Cl)(NPr_2)O$, 647-50
- Conformational effects on PNCH, PNC, and PNCi spin coupling in tervalent phosphorus-nitrogen compounds, 764-9
- Azomethine derivatives. Part 18. Diphenyl-, di-p-tolyl-, and di-tert-butyl-methyleneamino-derivatives of phosphorus, 986-9
- Crystal structure of 2,trans-4,cis-6,trans-8-tetrachloro-2,4,6,8-tetrakis(dimethylamino)cyclotetraphosphazene, 1094-8
- Acceptor properties of tetrachloro(phenyl)phosphorane and of the trichloro(phenyl)phosphonium ion, 1318-23
- Crystal structure of compounds with (N-P) $_n$ rings. Part 12. Decafluorocyclopentaphosphazene, 1425-30
- Reactions of some phosphorus(V) halides and halide oxides with strongly acidic solvents, 1455-60
- Acceptor properties of some o-phenylenedioxy-derivatives of phosphorus(V) chloride, 1465-71
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- PHOTOELEC SPECTRA**
- He(I) photoelectron spectra of tetracarbonyliron complexes of Group 5 ligands and of olefinic ligands, 695-8
- PHOTOELECTRON SPECTRA**
- Preparation and properties of some silyl- and germyl-

- halogenoacetylenes and of digermylacetylene, 759-63
 Photoelectron spectra of some transition metal alkyls and oxoalkyls 1403-7
 Photoelectron spectra of metal tetrahydroborates, 1755-61
 The electronic structure of magnesium dialuminium tetraoxide (spinel) using X-ray emission and X-ray photoelectron spectroscopies, 1785-90
 The electronic structure of magnesium hydroxide (brucite) using X-ray emission, X-ray photoelectron, and Auger spectroscopy, 1791-6
- PHOTOLYSIS**
 Photochemistry of carbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for trinitrosylmanganese, (dinitrogen)trinitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 202-7
 Photochemistry of tetracarbonylnitrosylmanganese in frozen gas matrices at 20 K. Infrared spectroscopic evidence for tricarbonylnitrosylmanganese, tricarbonyl(dinitrogen)nitrosylmanganese, and a species formed by metal-to-nitrosyl photoelectron transfer, 208-15
 Photochemical studies of the alkylammonium molybdates. Part 4. Electron spin resonance study of an irradiated single crystal of hexakis(isopropylammonium) dihydrogen octamolybdate dihydrate, 283-5
 Preparation and reactions of triphenylphosphine and triphenyl phosphite complexes of (benzylideneacetone)dicarbonyliron(0), 369-73
 The quenching of excited uranyl ion by d^6 metallocenes, 569-72
 Photochemistry of (η -benzene)tricarbonylchromium, tricarbonyl(η -cyclopentadienyl)manganese, and (η -cyclobutadiene)- and (trimethylenemethane)-tricarbonyliron in frozen gas matrices at 12 K. Infrared spectroscopic evidence for dicarbonylmetal and dicarbonyl(dinitrogen)metal complexes, 651-6
- PLATINUM**
 Unsaturated σ -hydrocarbyl transition-metal complexes. Part 4. Crystal and molecular structure of trans-chlorobis(diethylphenylphosphine)(phenylethynyl)platinum(II) and comments on the relative trans influence of various carbon ligands, 46-50
 A damped nonlinear least-squares computer program (DALFRK) for the evaluation of reaction rate constants, 123-31
 Optically active coordination compounds. Part 40. Mixed complexes of platinum(II) with L-proline and other α -amino-acids, 152-8
 Reactions of platinum(II) complexes. Part 2. Catalysis of the aquation of tetrachloroplatinate(II) ion by trichloro(η -ethylene)platinate(II) (Zeise's anion), 158-9
 Nickel, palladium, and platinum complexes of the ditertiary stibine 1,3-bis(dimethylstibino)propane, 177-80
 Complexes of platinum and palladium with tertiary dimethoxyphenylphosphines: attempts to effect O- or C-metallation, 257-62
 Monobridged binuclear platinum complexes. Part 1. Some phosphido-bridged diplatinum complexes of triethylphosphine, 272-6
 Synthesis and crystal structure of 3,3,4-tricyano-2,2-bis(triphenylphosphine)-1-oxa-2-platinacyclobutane, 279-82
 Oligomerization and telomerization of buta-1,3-diene catalyzed by bis(η -cycloocta-1,5-diene)-palladium and -platinum, 309-14
 Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
 Some binuclear hydrides of platinum, 516-22
 Kinetics of oxidation of dichlorobis(substituted pyridine)platinum(II) and of reduction of tetrachlorobis(substituted pyridine)platinum(IV) complexes, 699-702
 Displacement of chelate ligands from planar four-coordinate complexes. Part 5. Preparation and ligand-substitution reaction of dichloro(ethylenediamine)- and dichloro(propylenediamine)-gold(III) complexes, 728-34
 Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
 Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine) diplatinum complexes: crystal and molecular structure of di- μ -hydridobis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
 Preparation and vibrational spectra of tetra-n-propylammonium carbonyldichloro-organoplatinate(II) salts, and a comparison of their carbon-13 and platinum-195 nuclear magnetic resonance properties with those of organomercury compounds, 872-6
 Nuclear magnetic resonance studies of the addition of hydrogen halides to trans-cyanohydridobis(triethylphosphine)platinum(II) and hydridotris(triethylphosphine)platinum(II) tetraphenylborate 877-9
 Reactions of hexafluorobut-2-yne with alkylgold(I) complexes. Properties of intermediate binuclear gold(I)-gold(III) complexes, 980-5
 Complexes of platinum(II) with 2,2'-bipyrimidine: the effect of hydrogen bonding on intermetallic interactions, 1127-30
 Some palladium(II) and platinum(II) derivatives of pentaborane(9), 1146-52
 Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
 Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
 Platinum hydrides containing silyl or germyl ligands. Crystal structure of trans-hydridobis(tricyclohexylphosphine)platinum(II), 1167-70
 Metal complexes of sulphur ligands. Part 17. Reaction of palladium(II) and platinum(II) monothiobenzoates with various Lewis bases and further studies on complexes containing related ligands, 1195-200
 Use of aryltin compounds in the preparation of diaryl- and diaryldi- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
 Synthesis and dynamic behaviour of bis(ethylene)(tertiary phosphine)platinum complexes, 1337-42
 The structure of ac-dichloro-b-ethylene-d-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8
 Molecular and crystal structure of 3,3-bis(triethylphosphine)-1,2-dicarba-3-platnadodecaborane(11), and molecular orbital analysis of the slip distortion in carbametalaboranes, 1363-74
 Addition reactions on coordinated olefinic ligands. Part 8. Platinum(II) complexes of 1,1-dimethylallene and their reaction with amines. Molecular structure of the zwitterionic derivative dichloro(1-(NN-diethylammoniomethyl)-2-methylprop-1-enyl)(triphenylphosphine)platinum(II), 1392-7
 Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
 Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropenone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
 Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
 Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
 Electronic and resonance-Raman spectra of mixed-valence ammine complexes of palladium and platinum, 1622-7
 Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
 Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered anionic(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
 Some cyclopropylplatinum complexes, 1732-5
 Reactions of methylenecyclopropane with some hydridoplatinum(II) complexes, 1736-9
 The preparation, structures, and reactions of the metallocyclobutenyl complexes ($M_2(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
 Reaction of allene, 2,3-dimethylbuta-1,3-diene, and butadiene with bis(cycloocta-1,5-diene)-, bis(ethylene)(trimethylphosphine)-, and bis(ethylene)(tricyclohexylphosphine)platinum; crystal structures of η -cycloocta-1,5-diene- and bis(trimethylphosphine)(1,4-trans-divinylbutane-1,4-diyl)platinum, 1839-47
- POLYAMINE**
 Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10
 Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53

POLYMN

Transient intermediates in the polymerization of tungstate, 133-7

PRASEODYMIUM

Nuclear magnetic resonance studies of lanthanoid complexes. Part 3. Adducts of tris(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctane-3,5-dionato)praseodymium with bidentate amines, 315-19

Crystal structure of tetrakis- μ -trifluoroacetato-bis(triaqua(trifluoroacetato)praseodymium(III)), 1544-8

PROTONATION

Assignment of the proton-association constants for 3-(3,4-dihydroxyphenyl)alanine (L-dopa), 43-5

Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetonide complexes of rhodium and iridium, 50-3

Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10

The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms 228-34

Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53

Complexes of D-, L-, DL-, and meso-tartaric acid with hydrogen and oxovanadium(IV) cations, 286-90

Preparation of (η -cycloocta-1,5-diene) halogenohydrido-bis(phosphine)iridium(III) salts and kinetic study of the oxidative-addition reactions of (η -cycloocta-1,5-diene)bis(phosphine)iridium(I) salts with hydrohalogenic acids: evidence for anionic intermediates, 340-7

Protonation of the decavanadate(6-) ion: a vanadium-51 nuclear magnetic resonance study, 503-6

Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetraethylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92

Effect of mixed-ligand complex formation on the ionization of the pyrrole hydrogens of histamine and histidine, 964-8

Structural studies on biguanide and related species. Correlation of protonation energy with molecular structure, 989-96

Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarboylferrates and tricarboyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304

Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of ($M(C_5Me_5(sol)_3)(PF_6)_2$ ($M = Rh$ or Ir ; $sol = MeCN$, Me_2CO , or $MeOH$) with mono-, di-, and tri-olefins, 1305-11

Kinetics of the dissociation of decavanadate(6-) in neutral and weakly basic solutions, 1329-33

Reactions of some phosphorus(V) halides and halide oxides with strongly acidic solvents, 1455-60

Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropenone with platinum(0) complexes; crystal and molecular structure of μ -2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8

Reaction of tricarboyl(2-6- η -hexadienyl)iron with amines, triphenylphosphine, and triphenylarsine: a method for the preparation of triene complexes, 1678-82

Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76

PYRIDINE

Displacement of organic sulphides by amines in trans-dichlorobis(organic sulphide)palladium(II) complexes, 12-14

Crystal and molecular structure and some properties of pyridinium μ -oxobis(trichloroferrate(III))-pyridine, 80-4

Magnetic properties of hexakis(pyridine N-oxide)cobalt(II) perchlorate, 160-5

Crystal and molecular structures of (NN')-(2-(2'-pyridyl)ethyl)ethylenebis(salicylideneiminato)iron(II) and -cobalt(II)-ethanol (1/1), 185-91

Crystal and molecular structure of (dioxigen)(NN')-(2-(2'-pyridyl)ethyl)ethylenebis(salicylideneiminato)cobalt-acetonitrile (1/1), 191-6

The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms

228-34

Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7

Structure of (η -allyl)dicalbonyl(pentane-2,4-dionato)pyridinemolybdenum(II) in the solid and solution states, 291-5

Kinetics and mechanism of replacements in pentacyano(ligand)ferrate(II) ions. An attempt to distinguish between the D and I_d mechanisms, 500-2

Preparations and structures of NN'

-ethylenebis(salicylideneiminato)titanium(III) derivatives, 545-9

He(I) photoelectron spectra of tetracarbonyliron complexes of

Group 5 ligands and of olefinic ligands, 695-8

Kinetics of oxidation of dichlorobis(substituted pyridine)platinum(II) and of reduction of tetrachlorobis(substituted pyridine)platinum(IV) complexes, 699-702

Nitrosyl complexes of rhenium. Part 3. Crystal and molecular structure of tetraethylammonium tetrachloronitrosyl(pyridine)rhene(1-), 798-801

Preparation and characterization of a series of cationic monometallated, and neutral and cationic tridentate dimetallated, tri-o-tolyl phosphite iridium(III) complexes, 926-31

Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000

Kinetics of reactions of Schiff-base complexes of iron(II). Part 6.

The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8

Coordination bond properties in phthalocyaninatometal(II) complexes. Part 1. Stereochemistry and bond properties in

bis(4-methylpyridine)phthalocyaninatometal(II)-4-methylpyridine (1/2) (metal = cobalt or iron), 1018-24

Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9

Some mononuclear seven-coordinate rhenium(III) carbonyl complexes; the crystal and molecular structure of (2,2-bipyridyl)tribromodicarbonylrhenium(III), 1098-102

Some unusual iridium complexes formed from (2,6-dimethoxyphenyl)- and (2,3-dimethoxyphenyl)-di-tert-butylphosphine: crystal structure of (2-di-tert-butylphosphino-3-methoxyphenoxy-OP)(2-((2-hydroxy-6-methoxyphenyl)tert-butylphosphino)-2-methylpropano(2-)-C'IP(2))(methyl isocyanide)iridium(III), 1119-26

Preparation and structures of ruthenium(III) complexes containing tertiary arsines, tertiary phosphines, and isocyanides, 1152-4

Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60

Cobalt metallacycles. Part 5. Synthesis of pyridines from nitriles and acetylenes via cobaltacyclopentadienes, 1278-82

Reactions of tetracarbonylhydridoferrate(0) with acetylenes in aprotic solvents: (1-3- η -acryloyl)tricarboylferrates and tricarboyl(1-3- η -prop-2-en-1-ylidene)iron complexes, 1298-304

Acceptor properties of tetrachloro(phenyl)phosphorane and of the trichloro(phenyl)phosphonium ion, 1318-23

The structure of ac-dichloro-b-ethylene-d-pyridineplatinum(II) from hydrogen-1 and -2 nuclear magnetic resonance spectra of liquid-crystal solutions, 1355-8

Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4

Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl-N)palladium(II) perchlorate, 1490-6

Complexes of osmium(VI) with catechol and substituted catechols, 1501-6

Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602

Solvation effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6

Complexes of palladium(II) with nucleosides. Preparation and properties of complexes of the type potassium trichloro(nucleoside)palladate(II), 1691-5

Axial ligand dissociation of phthalocyaninatoiron(II) adducts.

- Further evidence for a dissociative mechanism of substitution, 1709-14
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide) aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- Allyl- and propadienyl-cobaloximes: character and reactions with tetracyanoethylene, 1814-20
- ### RADIOLYSIS
- Oxidation of first-row bivalent transition-metal complexes containing ethylenediaminetetraacetate and nitrilotriacetate ligands by free radicals. A pulse-radiolysis study, 1105-18
- ### RAMAN
- Resonance-Raman spectra of copper(II) and nickel(II) diethyldithiocarbamates, 53-6
- Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5
- Vapour-phase intensity studies of the Raman-active bands of Group 6 hexafluorides, 170-3
- Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
- Vibrational spectra of some trichloromethyl- and trifluoromethylmercury(II) compounds, 328-32
- Infrared and Raman spectroscopic studies of conformations in liquid and solid triethyl-, diethyl(methyl)- and ethyldimethylamines, -phosphines, and -arsines, 388-94
- Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6
- Solvation of mercury(II) halides and alkylmercury(II) halides by liquid ammonia: a Raman spectroscopic study, 705-10
- Molecular vibrations of zirconium(IV) tetrahydroborate, a compound containing triple hydrogen bridges, 710-22
- Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63
- Single-crystal infrared study and assignment for mercury(II) chloride and bromide, 776-82
- Single-crystal Raman and infrared study of aluminium trichloride hexahydrate, 782-8
- Group 3 tetrahydroborates. Part 1. The synthesis and properties of dimethylgallium tetrahydroborate, 809-17
- Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8
- Preparation and vibrational spectra of tetra- n -propylammonium carbonyldichloro-organoplatinate(II) salts, and a comparison of their carbon-13 and platinum-195 nuclear magnetic resonance properties with those of organomercury compounds, 872-6
- Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy 921-5
- Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43
- Derivatives of bivalent germanium, tin, and lead. Part 21. Tin(II) formate: a reinvestigation, 1274-8
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- Complexes of osmium(VI) with catechol and substituted catechols, 1501-6
- Synthesis and structure of some binuclear carbonyl complexes of platinum(I), 1540-4
- Studies of transition-metal oxo- and nitrido-complexes. Part 4. Reactions of osmium tetroxide with alkynes and dienes in the presence of tertiary amines, 1599-602
- Electronic and resonance-Raman spectra of mixed-valence ammine complexes of palladium and platinum, 1622-7
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- ### REDN
- Kinetics and mechanism of the reduction of thiocyanato-, isothiocyanato, and azido-pentaamminecobalt(III) by pentaammineaquaruthenium(II) in aqueous solutions, 148-51
- Preparation, structure, and redox properties of isocyanide complexes of molybdenum(0) and tungsten(0), 165-9
- Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
- Kinetics of oxidation of dichlorobis(substituted pyridine) platinum(II) and of reduction of tetrachlorobis(substituted pyridine)platinum(IV) complexes, 699-702
- Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
- Reaction of electrogenerated square-planar nickel(I) complexes with alkyl halides, 972-6
- The reaction between thallium(III) and hydrogen peroxide, 1012-17
- Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine) triisothiocyanatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
- Bis(tetrabutylammonium) tetrakis(benzenethiolato- μ_3 -selenido)iron, an iron-selenium cubic cluster compound, 1423-5
- ### RESONANCE RAMAN
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- ### RHENIUM
- Crystal structure of abcdc-pentacarbonyl- f - μ -fluoro-ghijk-pentafluororhenium(I)rhenium(V), 64-7
- Reactions of coordinated molecules. Part 9. Calculation of carbonyl stretching force constants of metallo-acetylacetonate molecules: evidence supporting intramolecular π bonding, 93-5
- Nitrosyl complexes of rhenium. Part 3. Crystal and molecular structure of tetraethylammonium tetrachloronitrosyl(pyridine) rhenate(1-), 798-801
- Structural studies of nitrido-complexes: X-ray crystal structure of tetraphenylarsonium pentakis(isothiocyanato)nitridorhenate(VI), 844-8
- Neutral, acetate-bridged, binuclear alkyls of rhenium(III), 1063-6
- Some mononuclear seven-coordinate rhenium(III) carbonyl complexes: the crystal and molecular structure of (2,2-bipyridyl) tribromodicarbonylrhenium(III), 1098-102
- Crystal and molecular structure of di- μ -bromo- μ -tetraphenyldiphosphane-bis(tricarbonylrhenium(I)), 1189-95
- Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine) triisothiocyanatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio) methanethiolato-bis(tricarbonylmanganese), 1247-55
- Photoelectron spectra of some transition metal alkyls and oxoalkyls 1403-7
- Studies on transition metal cyano complexes. Part 2. Unsubstituted cyanorhenates, $(\text{Re}(\text{CN})_5)^{2-}$, and cyanorhenates with thio-, seleno-, and nitrosyl ligands, 1411-17
- Rhenium carbonyl fluorides: preparation, crystal structure, and some properties of hexacarbonylrhenium(I) μ -fluoro-bis(pentafluororhenate(V)), 1627-31
- ### RHODIUM
- Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetylamine complexes of rhodium and iridium, 50-3
- Rhodium(I) complexes of diallyl ethers and related compounds, 333-9
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- New carbide clusters in the cobalt sub-group. Part 4. Synthesis and crystallographic characterization of μ_3 -carbonyl-deca- μ -carbonyl-dicarbido-tetradecacarbonyl-polyhydro-dodecarrhodium, 459-63
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and

- iridium with various dithioacid ligands, 486-95
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- Carbon-13 nuclear magnetic resonance spectra of polynuclear carbonyls of cobalt and rhodium, 626-34
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Trichloro-bridged heterobimetallic phosphine complexes containing ruthenium(II) and rhodium(III), 909-12
- Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 18. The reactions of $(M(C_5Me_5)(sol)_3)(PF_6)_2$ ($M = Rh$ or Ir ; $sol = MeCN, Me_2CO$, or $MeOH$) with mono-, di-, and tri-olefins, 1305-11
- Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di- μ -arythio-bis(η -cyclopentadienyl)rhodium), 1375-9
- Binuclear diaryltriazene- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- Structures of binary carbonyls and related compounds. Part 1. A new approach to fluxional behaviour, 1554-68
- Reactions of halo(phenyl)alkynes with complexes of platinum(0), palladium(0), rhodium(I), and iridium(I). Preparation of (1-2- η -chloro(phenyl)ethyne)bis(triphenylphosphine)platinum(0) and a chlororhodium(I) analog and the kinetics of isomerization of the former to an alkynyl complex, 1577-81
- Trans-influence of anionic, neutral, and bridging ligands on the nuclear magnetic resonance spectra of methyl- and fluorobenzyl-bis(dimethylglyoximate)rhodium(III) complexes. Some observations on bridge formation, 1807-13
- Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5
- RUBIDIUM**
- Crystal structures of octaccesium and octarubidium dicosaniobates 968-72
- RUTHENIUM**
- Ruthenium complexes containing Group 5B donor ligands. Part 5. Synthesis and crystal and molecular structure of acetone(carbonyl)chloro(trichlorostannio) bis(triphenylphosphine)ruthenium(II)-acetone (1/1), 76-9
- Schiff-base complexes of ruthenium(II), 110-15
- Kinetics and mechanism of the reduction of thiocyanato-, isothiocyanato, and azido-pentaamminecobalt(III) by pentaammineaquaruthenium(II) in aqueous solutions, 148-51
- Hydrocarbon complexes of iron, ruthenium, and osmium. 11.
- Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3-6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
- Crystal and molecular structure of μ -pentalenebis(dicarbonyl(trimethylgermyl)ruthenium), 412-16
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- The quenching of excited uranyl ion by d^6 metalocenes, 569-72
- Structural and mechanistic studies of coordination compounds. Part 21. Base hydrolysis of some trans-tetraaminedichlororuthenium(III) cations, 740-3
- Metal complexes of sulphur ligands. 16. Reaction of trichlorotris(dimethylphenylphosphine)ruthenium and dichlorotris(triphenylphosphine)ruthenium with sodium and ammonium monothiobenzoates; structure of (4-amino-2-imino-4-methylpentane)bis(dimethylphenylphosphine) bis(monothiobenzoato)ruthenium(II), 769-75
- Carbene complexes. 14. The synthesis, steric and electronic effects in electron-rich olefin-derived bis-, tris-, and tetrakis-(carbene) ruthenium(II) and a tetrakis(carbene)osmium(II) complex; crystal and molecular structure of trans-dichlorotetrakis(1,3-diethylimidazolidin-2-ylidene)ruthenium(II), 826-36
- Carbene complexes. Part 15. The synthesis and properties of electron-rich olefin-derived mono- and oligo-carbenitrosylruthenium, -osmium and -nickel complexes, 837-44
- Fluorophosphine complexes of ruthenium and osmium. Part 1. Syntheses and stereochemistry of dihydrido-complexes of ruthenium(II) and osmium(II), 885-9
- Fluorophosphine complexes of ruthenium and osmium. Part 2. Reactions of dihydrido-complexes with protic species, 889-95
- Fluorophosphine complexes of ruthenium and osmium. Part 3. Monomeric ruthenium(II) and osmium(II) halogeno-complexes, 895-901
- Fluorophosphine complexes of ruthenium and osmium. Part 4. Homobinuclear trichloro-bridged complexes of ruthenium(II), 901-9
- Trichloro-bridged heterobimetallic phosphine complexes containing ruthenium(II) and rhodium(III), 909-12
- Fluorophosphine complexes of ruthenium and osmium. Part 5. Alkene hydrogenation catalysed by ruthenium(II) complexes, 913-15
- Cationic ruthenium systems. Part 3. Preparation and characterization of cationic dienehydridotris(phosphine) ruthenium complexes. The crystal and molecular structure of (η -buta-1,3-diene)tris(dimethylphenylphosphine)hydridoruthenium(II) hexafluorophosphate, 1032-6
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridoruthenium with a series of neutral donor ligands, 1036-9
- Structural studies of substituted hydrazine complexes. Part 2. Crystal and molecular structure of (η -cyclo-octa-1,5-diene) tris(NN-dimethylhydrazine)hydridoruthenium(II) hexafluorophosphate, 1040-2
- Structural studies of substituted hydrazine complexes. Part 3. Crystal and molecular structure of dichlorobis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihydridoruthenium, an asymmetric triply bridged dimer containing a bidentate bridging NN-dimethylhydrazine ligand, 1043-6
- Preparation and structures of ruthenium(III) complexes containing tertiary arsines, tertiary phosphines, and isocyanides, 1152-4
- Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Organosulphur-transition metal chemistry. Part 4. The isomerism of μ -thio- and μ -seleno-bis(carbonyl(η -cyclopentadienyl) ruthenium) complexes, 1260-9
- Crystal and molecular structure of tri- μ -chloro-hexakis(trimethylsilylmethyl)-triangular-irithenium(III), 1334-7
- Formal Diels-Alder dimerization of cyclooctatetraene induced by carbonylruthenium complexes, 1514-23
- Reactions of dodecacarbonyl-triangular-irithenium and dodecacarbonyltetrahydrotetrairuthenium with mixtures of cyclic polyolefins, 1523-8
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- Bis(styrene)bis(triphenylphosphine)ruthenium(0) and its reactions with triphenylphosphine and with alkenes, 1739-45
- SCHIFF BASE**
- Schiff-base complexes of the lanthanoids and actinoids. Part 1. Lanthanoid(III) halide complexes with the unionized form of NN'-ethylenebis(salicylideneimine) and related bases, 36-9
- Schiff-base complexes of ruthenium(II), 110-15
- Crystal and molecular structures of (NN'-(2-(2'-pyridyl)ethyl) ethylenebis(salicylideneiminato))iron(II) and -cobalt(II)-ethanol (1/1), 185-91
- Crystal and molecular structure of (dioxigen)(NN'-(2-(2'-pyridyl) ethyl)ethylenebis(salicylideneiminato))cobalt-acetonitrile (1/1), 191-6
- Preparations and structures of NN'-ethylenebis(salicylideneiminato)titanium(III) derivatives, 545-9
- A classical polarizability treatment for planar bis(2-((R)-1,2,2-trimethylpropyliminomethyl)naphtholato(1-)-NO)nickel(II), 822-6
- Reaction of electrogenerated square-planar nickel(I) complexes with alkyl halides, 972-6
- Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6.

- The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- Structure and spectroscopic properties of bis(*N*-cyclohexyl-3-methoxysalicylideneiminato)copper(II), 1051-7
- The isomers of α -amino-acids with copper(II). Part 4. Catalysis of the racemization of optically active alanine by copper(II) and pyruvate in alkaline solution, 1444-7
- SELENIDE**
- Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
- SELENIUM**
- Vapour-phase intensity studies of the Raman-active bands of Group 6 hexafluorides, 170-3
- Crystal structure and absolute configuration of cobalt-doped α -hexafluoroantimonate(III) selenate, 977-80
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Organosulphur-transition metal chemistry. Part 4. The isomerism of μ -thio- and μ -seleno-bis(carbonyl(η -cyclopentadienyl) ruthenium) complexes, 1260-9
- Studies on transition metal cyano complexes. Part 2. Unsubstituted cyanorhenates, $(\text{Re}(\text{CN})_5)^-$, and cyanorhenates with thio-, seleno-, and nitrosyl ligands, 1411-17
- Bis(tetrabutylammonium) tetrakis(benzenethiolato- μ_3 -selenidoiron), an iron-selenium cubic cluster compound, 1423-5
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- SEMICONDUCTOR**
- Decentralized unpaired electrons and valence bonding in chromium uranium trisulphide, 1686-90
- SILICON**
- Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
- Hydrocarbon complexes of iron, ruthenium, and osmium. 11.
- Diruthenium complexes of pentalene derived from cyclooctatetraene: crystal and molecular structure of the fluxional molecule dicarbonyl(trimethylsilyl)(1-3,6-7- η -8-endo-trimethylsilylcyclooctatrienyl)ruthenium, a pentalene precursor, 403-12
- Metal-silacyclobutane complexes. Part 1. Derivatives of iron and manganese, 427-33
- Trimethylsilylmethyl and other alkyls of chromium, molybdenum, ruthenium, and rhodium from interaction of magnesium dialkyls with metal-metal bonded binuclear acetates of chromium(II), molybdenum(II), ruthenium(II, III), and rhodium(II), 446-53
- Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601
- Reactions of strained organosilicon heterocycles with nonacarbonyldiiron(0). Part 2. Preparation and reactions of silaferracyclopentanes, 665-73
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63
- Conformational effects on PNCH, PNC, and PNSi spin coupling in tervalent phosphorus-nitrogen compounds, 764-9
- Synthesis of trans-di- μ -hydrido-bis(silyl)bis(trialkylphosphine)diplatinum complexes: crystal and molecular structure of di- μ -hydridobis(tricyclohexylphosphine)bis(triethylsilyl)diplatinum, 801-8
- Stereochemically nonrigid silanes, germanes, and stannanes. Part 2. Silylcyclopentadienes, 938-43
- Organosilicon chemistry. Part 21. Reactions of NN-bis(trifluoromethylamino)-oxyl and perfluoro(2,4-dimethyl-3-oxa-2,4-diazapentane) with vinylsilanes, and pyrolysis of the resulting adducts, 1024-31
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- Platinum hydrides containing silyl or germyl ligands. Crystal structure of trans-hydridosilyl-bis(tricyclohexylphosphine)platinum(II), 1167-70
- Crystal and molecular structure of di- μ -trimethylsilylmethyl-bis(trimethylphosphine)chromium(II) (4Cr-Cr), 1314-18
- Crystal and molecular structure of tri- μ -chloro-hexakis(trimethylsilylmethyl)-triangulo-trirhenium(III), 1334-7
- Trimethylsilyl derivatives for the study of silicate structures. Part 5. Trimethylsilylation of diopside, 1342-9
- Reactions of silane with zeolitic water, 1746-52
- A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- SILVER**
- The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms 228-34
- Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
- Copper(I), silver(I), and gold(I) complexes with nido-pentaborane anions, 1144-5
- SODIUM**
- Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601
- SOLVENT**
- Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7
- SOLVENT EFFECT**
- Vibrational and nuclear magnetic resonance studies of the formation of alkylmercury(II) halide complex anions, 561-6
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 16. Homogeneous hydrogenation catalysts, 617-26
- Solvation of mercury(II) halides and alkylmercury(II) halides by liquid ammonia: a Raman spectroscopic study, 705-10
- Weak complexes of sulphur and selenium. Part 5. Halide-ion replacement in 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in acetonitrile and dimethyl sulphoxide, 915-18
- Weak complexes of sulphur and selenium. Part 6. Stability constants of the weak 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in the mixed solvent acetonitrile-dimethyl sulphoxide at 25°C, 918-20
- Reactions of low-spin iron(II) complexes with hydroxide ion in aqueous methanol: the effect of ligand on rates of reaction, 996-1000
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6. The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- Analysis of the effects of solvent on the initial and transition states in the kinetics of reaction between tris(1,10-phenanthroline)iron(II) cation and hydroxide ions in methanol- and acetone-water mixtures, 1086-90
- Solvation effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacetic ligands, 1647-53
- Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in aryldiazenedi(tris(dimethylthiocarbamate)molybdenum, 1654-8
- SOLVOLYSIS**
- Reactions of some phosphorus(V) halides and halide oxides with strongly acidic solvents, 1455-60
- SPINEL**
- The electronic structure of magnesium dialuminium tetraoxide (spinel) using X-ray emission and X-ray photoelectron spectroscopies, 1785-90
- STEREOCHEM**
- Stereochemistry of six-coordinate bis(tridentate ligand)metal complexes, 793-7
- STIBINE**
- Cationic ruthenium systems. Part 4. Bridge-splitting reactions of the triply bridged dimers bis(η -cyclo-octa-1,5-diene)(NN-dimethylhydrazine)dihalogenodihydridodiruthenium with a series of neutral donor ligands, 1036-9
- STRONTIUM**
- The organometallic chemistry of the alkaline-earth metals. Part 3. Preparation and properties of alkylhalogenometal compounds and related species of calcium, strontium, and barium, 657-64
- STRUCTURE**
- A potentially seven-coordinate complex that is only five-coordinate; crystal and molecular structure of di-iodo(6,7,8,9-

- tetrahydro-16,22-dimethyl-5,10-dithia-15,23,24-triaza-17,21-methenodibenzo(a,i)cyclononadecene-NN'N''zinc(II), 511-16
- Metal complexes of sesquidentate ligands derived from 3-ethoxymethylenepentane-2,4-dione. Reactions with aliphatic diamines and crystal structures of (3,3'-ethylenedithiois(phenyleneiminomethylidene)bis(pentane-2,4-dionato)(2-))-nickel(II) and -copper(II), 1057-62
- SUBSTITUTION**
- Displacement of organic sulphides by amines in trans-dichlorobis(organic sulphide)palladium(II) complexes, 12-14
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7
- Solvent effects on discrimination in the dissociative substitution of pentacyano(ligand)ferrate(II) complexes in alcohol-water mixtures, 244-7
- Kinetics of replacement of aminocarboxylates by macrocyclic polyamines in copper(II) complexes, 247-53
- Kinetics and mechanism of replacements in pentacyano(ligand)ferrate(II) ions. An attempt to distinguish between the D and I_d mechanisms, 500-2
- Displacement of chelate ligands from planar four-coordinate complexes. Part 5. Preparation and ligand-substitution reaction of dichloro(ethylenediamine)- and dichloro(propylenediamine)-gold(III) complexes, 728-34
- Reaction mechanisms of metal-metal-bonded carbonyls. Part 19. Homolytic fission of bis(tetracarbonyl(triphenylphosphine)manganese)(Mn-Mn) as a path for thermal substitution, 789-93
- Weak complexes of sulphur and selenium. Part 5. Halide-ion replacement in 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in acetonitrile and dimethyl sulphoxide, 915-18
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η-cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Complexes with sulphur and selenium donor ligands. Part 6. Kinetics and mechanism of the reaction between 1,2-bis(diphenylphosphino)ethane and tris(OO'-dimethyl phosphorodithioato)cobalt(III), 950-5
- Kinetics of reactions of Schiff-base complexes of iron(II). Part 6. The preparation and kinetics of reactions of complexes of multidentate ligands, 1001-8
- Chemistry of the metal carbonyls. Part 75. Synthesis of aquatetracarbonyl(triphenylphosphine)manganese tetrafluoroborate and related cationic tetracarbonylmanganese complexes, 1009-12
- Some four- and five-coordinate cations of platinum(II) containing alkylphosphine and hydride ligands, 1161-4
- Structural and mechanistic studies of coordination compounds. 22. Preparation and ligand-substitution kinetics of trans-dihalogeno- and trans-halogenoisothiocyanato-cobalt(III) complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-tetra-azabicyclo(11.3.1)-heptadeca-1(17),2,11,13,15-pentaene, 1180-5
- Kinetics and mechanisms of formation, and of reactions, of intermediates in the iron(II)-1,10-phenanthroline-cyanide and related systems, 1447-51
- Carbon-carbon double-bond cleavage in the reactions of diphenylcyclopropanone with platinum(0) complexes; crystal and molecular structure of μ-2-oxo-1,3-diphenylpropanediylidene-bis(bis(tert-butyl isocyanide)platinum), 1472-8
- Binuclear diaryltriazenido- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- Solvation effects on the kinetics of diamine replacement in pentacyano(diamine)ferrate(II) complexes, 1603-6
- Fast reactions at planar four-coordinate complexes. Part 3. Kinetics and mechanism of substitution reactions of sterically hindered anionic(mesityl)bis(triethylphosphine)nickel(II) complexes, 1682-5
- Axial ligand dissociation of phthalocyaninatoiron(II) adducts. Further evidence for a dissociative mechanism of substitution, 1709-14
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- Rates and activation parameters for the stepwise formation of mono complexes of the hexakis(dimethyl sulphoxide)aluminium(III) ion with uni-, bi-, and ter-dentate nitrogen-donor ligands in nitromethane solution, 1776-81
- Reactions of allyl- and propadienyl-rhodium(III) and -iridium(III) complexes with polyhalogenomethanes. Rhodium(II) and iridium(II) species as reactive intermediates, 1821-5
- SULPHIDE**
- Displacement of organic sulphides by amines in trans-dichlorobis(organic sulphide)palladium(II) complexes, 12-14
- Chalcogen derivatives of iron carbonyls. Part 7. Kinetics and mechanism of carbonyl replacement in a nonacarbonylthiodicobaltiron, 222-7
- Hydrides of platinum(II) and platinum(IV) incorporating hydrogen sulphide and hydrogen selenide ligands, 753-8
- Single-crystal molecular and electronic structure of trichlorooxo(triphenylphosphine sulphide)molybdenum(V), 1350-4
- Decentralized unpaired electrons and valence bonding in chromium uranium trisulphide, 1686-90
- SULPHUR**
- Vapour-phase intensity studies of the Raman-active bands of Group 6 hexafluorides, 170-3
- A theoretical investigation of the structure of some small nitrogen-sulphur molecules, 277-9
- Electron-diffraction investigation of the molecular structure of sulphonyl chloride isocyanate, 299-302
- Crystal and molecular structure of the polymeric complex chloro(2,5-dithiahexane)copper(I), 416-18
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η-arene)dichlororuthenium and bis(dichloro(η-pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- ⁵⁷Fe-¹A₁ transitions in six-coordinate iron(II) complexes of 2,2'-bi-2-thiazoline and 2,2'-bi-4,5-dihydrothiazine ligands, 522-6
- Kinetics and mechanism of the sulphamic acid-nitric acid reaction: evidence for consecutive reactions, 530-4
- Sulphur-nitrogen compounds. Part 5. The oxidation of N-aryl-N-(arylsulphonyl)hydroxylamines: preparation of N-aryl-NO-bis(arylsulphonyl)hydroxylamines, 604-7
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Molecular structure of divinyl sulphone as studied by electron diffraction, vibrational spectroscopy, and semiempirical CNDO/2 molecular-orbital calculations, 861-8
- Weak complexes of sulphur and selenium. Part 5. Halide-ion replacement in 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in acetonitrile and dimethyl sulphoxide, 915-18
- Weak complexes of sulphur and selenium. Part 6. Stability constants of the weak 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in the mixed solvent acetonitrile-dimethyl sulphoxide at 25°C, 918-20
- Torsional vibrations in some sulphur-nitrogen compounds studied by inelastic neutron scattering, infrared, and Raman spectroscopy 921-5
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di-μ-N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Organosulphur-transition metal chemistry. Part 4. The isomerism of μ-thio- and μ-seleno-bis(carbonyl(η-cyclopentadienyl)ruthenium) complexes, 1260-9
- Reduction-oxidation properties of organotransition metal complexes. Part 6. The isomerization, and one-electron oxidation, of syn- and anti-di-μ-arylthio-bis(η-cyclopentadienyl)rhodium, 1375-9
- Reactions of metal carbonyl derivatives. Part 22. The crystal and molecular structures of dicarbonyl(η-cyclopentadienyl)(ethylthio)iron and μ-ethylthio-bis(dicarbonyl(η-cyclopentadienyl)iron) tetrafluoroborate, and a comparison of their molecular parameters, 1379-85
- Studies on transition metal cyano complexes. Part 2. Unsubstituted cyanorhenates, (Re(CN)₅)⁰⁻, and cyanorhenates with thio-, seleno-, and nitrosyl ligands, 1411-17
- Bis(tetraethylammonium) tetrakis(benzenethiolato-μ₃-selenido)iron, an iron-selenium cubic cluster compound, 1423-5
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- Reactions of some phosphorus(V) halides and halide oxides with

- strongly acidic solvents, 1455-60
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine) molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Reactions between copper(II) and 2-mercaptopropionic acid in aqueous perchlorate solution, 1606-9
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- Inorganic heterocycles. The reaction of 1,1'-bis(1-phospholan-1-thione) with some transition-metal salts, 1662-3
- Versatility of the coordination behaviour of 1-methylpyrimidine-2-thione towards metal ions of the first transition series, 1705-9
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- Crystal structure of trichlorosulphonium(IV) tetrachloroiodate(III), 1723-5
- TANTALUM**
- Photoelectron spectra of some transition metal alkyls and oxoalkyls 1403-7
- TARTARIC**
- Complexes of D-, L-, DL-, and meso-tartaric acid with hydrogen and oxovanadium(IV) cations, 286-90
- TECHNETIUM**
- Carbonyltrichlorotris(dimethylphenylphosphine)technetium-ethanol (1/1), the first seven-coordinate complex of technetium; position of this molecule in the C_{3v} family, 373-80
- TELLURIUM**
- Vapour-phase intensity studies of the Raman-active bands of Group 6 hexafluorides, 170-3
- Reactions of tellurium oxides with alkali-metal oxides and hydroxides, 948-50
- Negative-ion mass spectra of trinuclear carbonyl clusters, 1164-6
- Crystal structure of dilaed tritellurate(IV), 1528-32
- TETRAHYDROBORATE**
- Photoelectron spectra of metal tetrahydroborates, 1755-61
- THALLIUM**
- Hydrogen-1 nuclear magnetic resonance evidence for trans addition in oxhyallation of acyclic olefins, 234-7
- The reaction between thallium(III) and hydrogen peroxide, 1012-17
- THERMODYNAMICS**
- Thermodynamics of extraction equilibria. Part 5. Correction of the method for the determination of equilibrium constants of extraction processes, 1-4
- Assignment of the proton-association constants for 3-(3,4-dihydroxyphenyl)alanine (L-dopa), 43-5
- Effects of cyclization and ring size on complex formation between penta-amine ligands and copper(II), 104-10
- A damped nonlinear least-squares computer program (DALSEK) for the evaluation of equilibrium constants from spectrophotometric and potentiometric data, 115-23
- The linear free-energy relation in the thermodynamics of complex formation. Part 2. Analysis of the formation constants of complexes of the large metal ions silver(I), mercury(II), and cadmium(II) with ligands having 'soft' and nitrogen-donor atoms 228-34
- Complexes of D-, L-, DL-, and meso-tartaric acid with hydrogen and oxovanadium(IV) cations, 286-90
- Standard enthalpies of formation of tris(bis(pentane-2,4-dionato)nickel(II)) and bis(2,2,6,6-tetramethylheptane-3,5-dionato)nickel(II) and an estimation of nickel-oxygen bond energies, 399-402
- Thermodynamics of metal complex formation in aqueous melts of calcium dinitrate-ammonium nitrate. Part 2. Cadmium(II) bromides, 549-52
- A microcalorimetric study of the macrocyclic effect. Enthalpies of formation of copper(II) and zinc(II) complexes with some tetra-aza macrocyclic ligands in aqueous solution, 577-83
- Mixed-ligand complexes of palladium(II). Part 3. Diaqua(ethylenediamine)palladium(II) complexes of L-amino-acids, 726-8
- Weak complexes of sulphur and selenium. Part 5. Halide-ion replacement in 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in acetonitrile and dimethyl sulphoxide, 915-18
- Weak complexes of sulphur and selenium. Part 6. Stability constants of the weak 1:1 complexes of sulphur dioxide, thionyl chloride, and sulphonyl chloride with halide ions in the mixed solvent acetonitrile-dimethyl sulphoxide at 25°C, 918-20
- Structural studies on biguanide and related species. Correlation of protonation energy with molecular structure, 989-96
- Equilibria of complex formation between several bivalent metal ions and macrocyclic tri- and penta-amines, 1081-5
- Thermodynamic and spectroscopic properties of mixed complexes in aqueous solution. Copper(II) complexes of 2,2'-bipyridyl and dicarboxylic acids, 1090-4
- Thermochemistry of dichlorobis(triphenylphosphine oxide)-zinc(II)-cadmium(II), and -mercury(II), 1102-4
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- A kinetic study of the formation of some unchelated and chelated beryllium(II) complexes in aqueous solutions, 1221-5
- Interaction of vitamin B₁₂ with 8-azaguanine and 6-mercaptopurine: kinetic and thermodynamic characterizations, 1226-32
- Comparison of the structure and dynamic properties of anion(1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) perchlorate complexes in nitromethane solutions, and the crystal and molecular structure of the chloro complex, 1282-8
- The standard enthalpies of formation of tris(pentane-2,4-dionato)molybdenum(III) and dioxobis(pentane-2,4-dionato)molybdenum(VI), and the molybdenum-pentane-2,4-dionate bond-enthalpy contributions, 1311-13
- Synthesis and dynamic behaviour of bis(ethylene)(tertiary phosphine)platinum complexes, 1337-42
- Computer simulation of metal-ion equilibria in biofluids. Part 2. Formation constants for zinc(II)-citrate-cysteine binary and ternary complexes and improved models of low-molecular-weight zinc species in blood plasma, 1433-8
- Empirical force-field calculations of strain-energy contributions to the thermodynamics of complex formation. Part 1. The difference in stability between complexes containing five- and six-membered chelate rings, 1438-44
- Aspects of the thermal decomposition of ϵ -zinc hydroxide: a kinetic compensation effect, 1484-9
- Comparison of 8-methylquinoline and benzo(h)quinoline complexes of palladium(II) with those of related ligands. Crystal and molecular structure of aqua(benzo(h)quinoline)(2-(dimethylaminomethyl)phenyl-N)palladium(II) perchlorate, 1490-6
- Solvent-exchange kinetics in nickel(II) solutions of aqueous tris(dimethylamino)phosphine oxide studied by pulsed phosphorus-31 nuclear magnetic resonance spectroscopy, 1506-10
- A carbon-13 nuclear magnetic resonance investigation of the ring exchange in (1-4- η^6 -cyclooctatetraene)(1-6- η^6 -cyclooctatetraene)iron, 1761-6
- The preparation, structures, and reactions of the metallocyclobutene complexes ($M_3(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropene salts to zerovalent palladium and platinum compounds, 1830-9
- THF**
- Alkyl-arene and -cyclooctadiene complexes of molybdenum(II) containing tertiary phosphines, 1139-43
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- Crystal and molecular structure of di- μ -bromo- μ -tetraphenyldiphosphane-bis(tricarbonylrhenium(I)), 1189-95
- THIOACID**
- Metal complexes of sulphur ligands. 16. Reaction of trichlorotris(dimethylphenylphosphine)ruthenium and dichlorotris(triphenylphosphine)ruthenium with sodium and ammonium monothiobenzoates; structure of (4-amino-2-imino-4-methylpentane)bis(dimethylphenylphosphine)bis(monothiobenzoato)ruthenium(II), 769-75
- Metal complexes of sulphur ligands. Part 17. Reaction of palladium(II) and platinum(II) monothiobenzoates with various Lewis bases and further studies on complexes containing related ligands, 1195-200
- THIOCARBAMATE**
- Resonance-Raman spectra of copper(II) and nickel(II) diethyldithiocarbamates, 53-6
- The chemistry of cyclopentadienyl nitrosyl and related complexes of molybdenum. Part 7. The fluxional behaviour of bis(cyclopentadienyl)dithiocarbamatomolybdenum complexes,

- and the application of Forsen-Hoffman spin-saturation method to the nuclear magnetic resonance spectra of a five-spin system, 467-74
- The chemistry of cyclopentadienyl nitrosyl and related molybdenum complexes. Part 9. Reactions of bis(cyclopentadienyl) complexes with dienophilic acetylenes and olefins, 480-2
- Metal complexes of sulphur ligands. Part 15. Reaction of bis(η -arene)dichlororuthenium and bis(dichloro(η -pentamethylcyclopentadienyl)metal) complexes of rhodium and iridium with various dithioacid ligands, 486-95
- Pentamethylcyclopentadienyl-rhodium and -iridium complexes. Part 17. Complexes with sulphur-containing ligands, 849-57
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Studies in eight-coordination. Part 5. Crystal and molecular structure and electron spin resonance spectra of tetrakis(diethylthiocarbamato)molybdenum(V) hexamolybdate and chloride, 1582-9
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- Proton nuclear magnetic resonance study of electronic transmission effects and fluxional behaviour in arylidiazeneidotrakis(dimethylthiocarbamato)molybdenum, 1654-8
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- The preparation, structures, and reactions of the metallaacyclobutenyl complexes ($M_2(C_3R^1R^2)_2X_2$) derived from addition of triarylcyclopropenium salts to zerovalent palladium and platinum compounds, 1830-9
- THIOCARBONATE**
Organosulphur-transition metal chemistry. Part 1. Reactions of carbon disulphide with metal carbonyl anions, 1240-6
- Metal complexes of sulphur ligands. Part 18. Reaction of tris- and tetrakis-(tertiary phosphine)dichlororuthenium(II) complexes with various dithioacid ligands, 1647-53
- THIOCYANATE**
Structural studies of nitrido-complexes: X-ray crystal structure of tetraphenylarsonium pentakis(isothiocyanato)nitridorhenate(VI), 844-8
- Structural and mechanistic studies of coordination compounds. 22. Preparation and ligand-substitution kinetics of trans-dihalogeno- and trans-halogenoisothiocyanato-cobalt(III) complexes of 2,12-dimethyl- and 2,7,12-trimethyl-3,7,11,17-tetra-azabicyclo(1.3.1)-heptadeca-1(17),2,11,13,15-pentaene, 1180-5
- Crystal and molecular structure of the complex (1,2-bis(diphenylphosphino)ethane)(diethylphenylphosphine)triisothiocyanatorhenium(III) and the electrochemistry of isothiocyanato-derivatives of rhenium(III) and rhenium(IV), 1232-6
- Organosulphur-transition metal chemistry. Part 2. Reactions of isothiocyanates with metal carbonyl anions: crystal and molecular structure of di- μ -N-methylimino(methylthio)methanethiolato-bis(tricarbonylmanganese), 1247-55
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- Crystal structures of the benzo-15-crown-5 complexes diisothiocyanato(2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin)magnesium, -calcium-methanol (1/1), and -calcium hydrate, 1418-23
- Complexes of palladium(II) and platinum(II) thiocyanates with some bidentate amine, phosphine, arsine, sulphide, and selenide ligands, 1460-4
- Complexes with sulphur and selenium donor ligands. Part 8. Some 4-phenylthiosemicarbazone complexes of cobalt(II) and the crystal structure of bis(acetone 4-phenylthiosemicarbazone) cobalt(II) bromide (green form), 1549-54
- The structure of tin(II) thiocyanate, 1797-9
- THIOPHOSPHATE**
A nuclear magnetic resonance investigation of bis(OO'-diethyl dithiophosphato)-complexes of the lanthanoids: separation of contact and pseudo-contact contributions to the chemical shifts, 267-72
- THIOPHOSPHINATE**
Preparation and characterization of dithiophosphinato-complexes of yttrium and the lanthanoids, 85-90
- THIOSEMICARBAZIDE**
X-ray crystal structures of μ -chloro-(tris(trichloro(thiosemicarbazide)bismuth(III))) (tris(thiosemicarbazide)bismuth(III)) hexachlorobismuthate(III) chloride and catena- μ -chloro-dichlorobis(ethylenethiourea)bismuth(III), 583-7
- THIOSEMICARBAZONE**
Complexes with sulphur and selenium donor ligands. Part 8. Some 4-phenylthiosemicarbazone complexes of cobalt(II) and the crystal structure of bis(acetone 4-phenylthiosemicarbazone) cobalt(II) bromide (green form), 1549-54
- THIOUREA**
X-ray crystallographic studies on ferrocene included in a thiourea host lattice, 15-18
- THORIUM**
Trimethylphosphine oxide complexes of thorium and uranium tetraniates; crystal structures of ten- and twelve-coordinate complex ions, bis(trinitratotetrakis(trimethylphosphine oxide)thorium(IV)) hexanitratothorate(IV) and tetraphenylphosphonium pentanitratobis(trimethylphosphine oxide)thorate(IV), 638-46
- TIN**
Ruthenium complexes containing Group 5B donor ligands. Part 5. Synthesis and crystal and molecular structure of acetone(carbonyl)chloro(trichlorostannio) bis(triphenylphosphine)ruthenium(II)-acetone (1/1), 76-9
- Coordinative tin-oxygen interactions in dinitratodiphenyl(triphenylphosphine oxide)tin(IV), 131-3
- Preparation of arylplatinum(II) complexes. The interaction of dichloro(η -cycloocta-1,5-diene)platinum(II) and aryltrimethylstannanes, 357-68
- The crystal structure of tin(II) bis(dihydrogenphosphate), 566-9
- Derivatives of bivalent germanium, tin, and lead. Part 21. Tin(II) formate: a reinvestigation, 1274-8
- Use of aryltin compounds in the preparation of diaryl- and diaroyl-di- μ -chloro-bis(triorganophosphine)diplatinum(II) complexes, 1288-94
- Reactions in mixed non-aqueous systems containing sulphur dioxide. Part 1. The dissolution of main-group metals in the binary mixture dimethyl sulphoxide-sulphur dioxide, 1431-3
- The structure of tin(II) thiocyanate, 1797-9
- TITANIUM**
Reactions of dichlorodiphenoxotitanium(IV), 454-9
- Preparations and structures of NN'-ethylenebis(salicylideneiminato)titanium(III) derivatives, 545-9
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Crystal and molecular structure of trichloro(2,5,8-trioxanonane)titanium(III), 1176-9
- Structure and properties of carbonylbis(η -cyclopentadienyl)(η -diphenylacetylene)titanium: the first titanium complex containing a two-carbon η -bonded ligand, 1398-403
- TRANS EFFECT**
Unsaturated σ -hydrocarbyl transition-metal complexes. Part 4. Crystal and molecular structure of trans-chlorobis(diethylphenylphosphine)(phenylethynyl)platinum(II) and comments on the relative trans influence of various carbon ligands, 46-50
- TRIAZACYCLODODECENE**
Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); X-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II), 68-76
- TRIAZENE**
Cationic diaryltriazene, hydrido(diaryltriazenido)-, and diarylacetamidine complexes of rhodium and iridium, 50-3
- TRIAZENIDE**
Binuclear diaryltriazenido- and aryl(1-aryliminoethyl)amido-complexes of rhodium, 1532-6
- TUNGSTATE**
Transient intermediates in the polymerization of tungstate, 133-7
- TUNGSTEN**
Transient intermediates in the polymerization of tungstate, 133-7

- Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
- Preparation, structure, and redox properties of isocyanide complexes of molybdenum(0) and tungsten(0), 165-9
- Solid-state studies. Part 11. The vibrational spectra of mixed crystals of tricarbonyl(η -mesitylene)-chromium, -molybdenum, -tungsten in the 2000 cm^{-1} region, 262-7
- Oxygen exchange between oxo-anions and water in basic media: molybdate(2-) and tungstate(2-), 496-500
- Unidentate sulphur-bonded monothio- β -diketone complexes of chromium(0), molybdenum(0), and tungsten(0) and their protonation. The X-ray structure analysis of tetrathylammonium pentacarbonyl(1,1,1-trifluoro-4-(2-thienyl)-4-thioxobutan-2-onato-S)tungstate(0), 587-92
- Synthesis of cationic carbonyl cyclopentadienyl complexes of molybdenum and tungsten, and X-ray crystal structure of (acetone hydrazone)tricarbonyl(η -cyclopentadienyl)tungsten hexafluorophosphate, 932-7
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80
- Organosulphur-transition metal chemistry. Part 3. Methyl thiocyanate complexes: crystal and molecular structure of pentacarbonyl(methyl thiocyanate)chromium, 1255-60
- Photoelectron spectra of some transition metal alkyls and oxoalkyls 1403-7
- Mechanism of alkylation and acylation of dinitrogen coordinated to molybdenum and tungsten, 1638-47
- Dealkylation of chelating ethers by reaction with WCl_4Y ($\text{Y} = \text{O}, \text{S}, \text{Se}, \text{or } \text{NC}_2\text{Cl}_3$), 1658-61
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- Hydrazido(2-)-complexes of molybdenum and tungsten formed from dinitrogen complexes by protonation and ligand exchange, 1766-76
- A comparison of the base decomposition of 12-tungstophosphate(3-), 12-tungstosilicate(4-), 12-tungstoborate(5-), and dihydrogendodecatungstate(6-), 1781-4
- ### TUNGSTOSILICATE
- Stepwise base decomposition of 12-tungstosilicate(4-), 137-41
- ### URANIUM
- Some oxygen-donor complexes of cyclopentadienyluranium(IV) halides, 295-8
- Co-condensation reactions of uranium tetrafluoride and hexafluoride with alkali metals and alkali-metal fluorides in low-temperature argon matrices, 433-40
- The quenching of excited uranyl ion by d^6 metallocenes, 569-72
- The chemistry of uranium. Part 20. Tetraphenylphosphonium pentachloro-oxouranate(IV): crystal structure and bonding characteristics, 592-7
- Trimethylphosphine oxide complexes of thorium and uranium tetranitrates; crystal structures of ten- and twelve-coordinate complex ions, bis(trinitratotetrakis(trimethylphosphine oxide)thorium(IV)) hexanitratothorate(IV) and tetraphenylphosphonium pentanitratobis(trimethylphosphine oxide)thorate(IV), 638-46
- Crystal and molecular structure of dichlorodioxobis(triphenylphosphine oxide)uranium(VI), 677-80
- Preparation, properties, and crystal structure of tetraethylammonium bis(1,3-diphenylpropane-1,3-dionato)nitratodioxouranate(VI), 818-21
- Preparation and physicochemical characterization of anionic uranyl β -ketoenolates, 1618-21
- Decentralized unpaired electrons and valence bonding in chromium uranium trisulphide, 1686-90
- Photoelectron spectra of metal tetrahydroborates, 1755-61
- ### UV
- Gold complexes of L-cysteine and D-penicillamine, 199-201
- The magnetic circular-dichroism spectrum of matrix-isolated vanadium hexacarbonyl, 608-11
- Preparation and properties of some silyl- and germyl-halogenoacetylenes and of digermylacetylene, 759-63
- A classical polarizability treatment for planar bis(2-(R)-1,2,2-trimethylpropyliminomethyl)naphtholato(1-)-NO nickel(II), 822-6
- Complexes with sulphur and selenium donor ligands. Part 7. The crystal and molecular structure of bis(diphenylphosphinodithioato)cobalt(II)-quinoline(1/1), 956-9
- Thermodynamic and spectroscopic properties of mixed complexes in aqueous solution. Copper(II) complexes of 2,2'-bipyridyl and dicarboxylic acids, 1090-4
- Magnetic susceptibility and optical spectra of the organic-intercalated two-dimensional ferromagnets bis(monomethylammonium)- and bis(monothethylammonium) tetrachlorochromate(II), 1207-12
- X-ray crystal-structure analysis and magnetic and spectral properties of tetrachlorotris(dichloro(methyl)phosphine) molybdenum(IV)-carbon disulphide (3/1), 1536-40
- Studies in eight-coordination. Part 5. Crystal and molecular structure and electron spin resonance spectra of tetrakis(diethyldithiocarbamate)molybdenum(V) hexamolybdate and chloride, 1582-9
- ### VALENCE BONDING
- Decentralized unpaired electrons and valence bonding in chromium uranium trisulphide, 1686-90
- ### VANADIUM
- Electron spin resonance studies of Ziegler-type catalysts. Part 2. Identification and spectra of some dialkylid(η -cyclopentadienyl) vanadium(IV) complexes, 57-61
- Complexes of D-, L-, DL-, and meso-tartaric acid with hydrogen and oxovanadium(IV) cations, 286-90
- Electron spin resonance spectra of trigonal-prismatic bis(pentane-2,4-dione benzoylhydrazonato(2-))vanadium(IV) and bis(4-phenylbutane-2,4-dione benzoylhydrazonato(2-))vanadium(IV), 423-6
- Protonation of the decavanadate(6-) ion: a vanadium-51 nuclear magnetic resonance study, 503-6
- The magnetic circular-dichroism spectrum of matrix-isolated vanadium hexacarbonyl, 608-11
- Kinetics and mechanism of redox reactions in aqueous solution. Part 2. Oxidation of phosphorous acid by vanadium(V) ion, 681-6
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Kinetics of the dissociation of decavanadate(6-) in neutral and weakly basic solutions, 1329-33
- Resonance-Raman spectroscopy of tris(1,2-dithiolene) complexes of vanadium, molybdenum, and tungsten, 1714-21
- ### VINYL KETONE
- Formation of η^3 -bonded lactone complexes and eight-membered ring metallacycles with ketene groups by the insertion of acetylenes into carbon-molybdenum and -tungsten σ bonds; molecular and crystal structures of products derived from $\text{MoMe}(\text{CO})_3(\eta\text{-C}_3\text{H}_5)$ and but-2-yne, 1067-80
- ### VITAMIN B12A
- Interaction of vitamin B_{12a} with 8-azaguanine and 6-mercaptopurine: kinetic and thermodynamic characterizations, 1226-32
- ### WILLEMITE
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- ### YLIDE
- Reactions of 2-azidopyridine and 1-pyridinio ylides with transition metal complexes, 1155-60
- ### YTTRIUM
- Preparation and characterization of dithiophosphinato-complexes of yttrium and the lanthanoids, 85-90
- ### ZEOLITE
- Hydrothermal chemistry of silicates. Part 22. Hydrated barium-sodium aluminosilicates, 598-601
- Reactions of silane with zeolitic water, 1746-52
- ### ZINC
- A potentially seven-coordinate complex that is only five-coordinate: crystal and molecular structure of di-iodo(6,7,8,9-tetrahydro-16,22-dimethyl-5,10-dithia-15,23,24-triaza-17,21-methenodibenzo(a,j)cyclononadecene-NN'N'')zinc(II), 511-16
- A microcalorimetric study of the macrocyclic effect. Enthalpies of

- formation of copper(II) and zinc(II) complexes with some tetra-aza macrocyclic ligands in aqueous solution, 577-83
- Complexes of pyrimidine-2-thione with some bivalent metal halides of the first transition series, 880-4
- Effect of mixed-ligand complex formation on the ionization of the pyrrole hydrogens of histamine and histidine, 964-8
- Crystal structure and absolute configuration of cobalt-doped α -hexaaquazinc(II) selenate, 977-80
- Trimethylsilyl derivatives for the study of silicate structures. Part 4. The conversion of hemimorphite into willemite, 1134-8
- Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, 1269-73
- Comparison of the structure and dynamic properties of aniono(1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)zinc(II) perchlorate complexes in nitromethane solutions, and the crystal and molecular structure of the chloro complex, 1282-8
- Computer simulation of metal-ion equilibria in biofluids. Part 2. Formation constants for zinc(II)-citrate-cysteinate binary and ternary complexes and improved models of low-molecular-weight zinc species in blood plasma, 1433-8
- Aspects of the thermal decomposition of ϵ -zinc hydroxide: a kinetic compensation effect, 1484-9
- ### ZIRCONIUM
- Molecular vibrations of zirconium(IV) tetrahydroborate, a compound containing triple hydrogen bridges, 710-22
- Silylmethyl and related complexes. Part 6. Preparation, properties, and crystal and molecular structure of tris(bis(trimethylsilyl)methyl)chromium(III); the chemistry of related compounds of titanium(III), vanadium(III), zirconium(IV), and hafnium(IV), 734-40
- Photoelectron spectra of metal tetrahydroborates, 1755-61
- ### ZWITTERION
- Addition reactions on coordinated olefinic ligands. Part 8. Platinum(II) complexes of 1,1-dimethylallene and their reaction with amines. Molecular structure of the zwitterionic derivative dichloro(1-(NN-diethylammoniomethyl)-2-methylprop-1-enyl)(triphenylphosphine)platinum(II), 1392-7

The first of these is the fact that the medical profession is not a homogeneous group. There are many different types of physicians, each with his own special interests and concerns. The second is the fact that the medical profession is not a monolithic entity. It is made up of many different groups, each with its own voice and its own interests. The third is the fact that the medical profession is not a static entity. It is constantly changing and evolving, and it is constantly being challenged by new ideas and new technologies.

The fourth is the fact that the medical profession is not a self-regulating body. It is subject to the same laws and regulations as any other profession, and it is subject to the same scrutiny and oversight. The fifth is the fact that the medical profession is not a closed shop. It is open to anyone who is qualified to practice medicine, and it is open to anyone who is interested in the health of the community.

The sixth is the fact that the medical profession is not a monopoly. It is a profession that is open to competition, and it is a profession that is subject to the same market forces as any other profession. The seventh is the fact that the medical profession is not a cartel. It is a profession that is subject to the same laws and regulations as any other profession, and it is subject to the same scrutiny and oversight.

The eighth is the fact that the medical profession is not a guild. It is a profession that is open to anyone who is qualified to practice medicine, and it is open to anyone who is interested in the health of the community. The ninth is the fact that the medical profession is not a cartel. It is a profession that is subject to the same laws and regulations as any other profession, and it is subject to the same scrutiny and oversight.

The tenth is the fact that the medical profession is not a cartel. It is a profession that is subject to the same laws and regulations as any other profession, and it is subject to the same scrutiny and oversight. The eleventh is the fact that the medical profession is not a cartel. It is a profession that is subject to the same laws and regulations as any other profession, and it is subject to the same scrutiny and oversight.

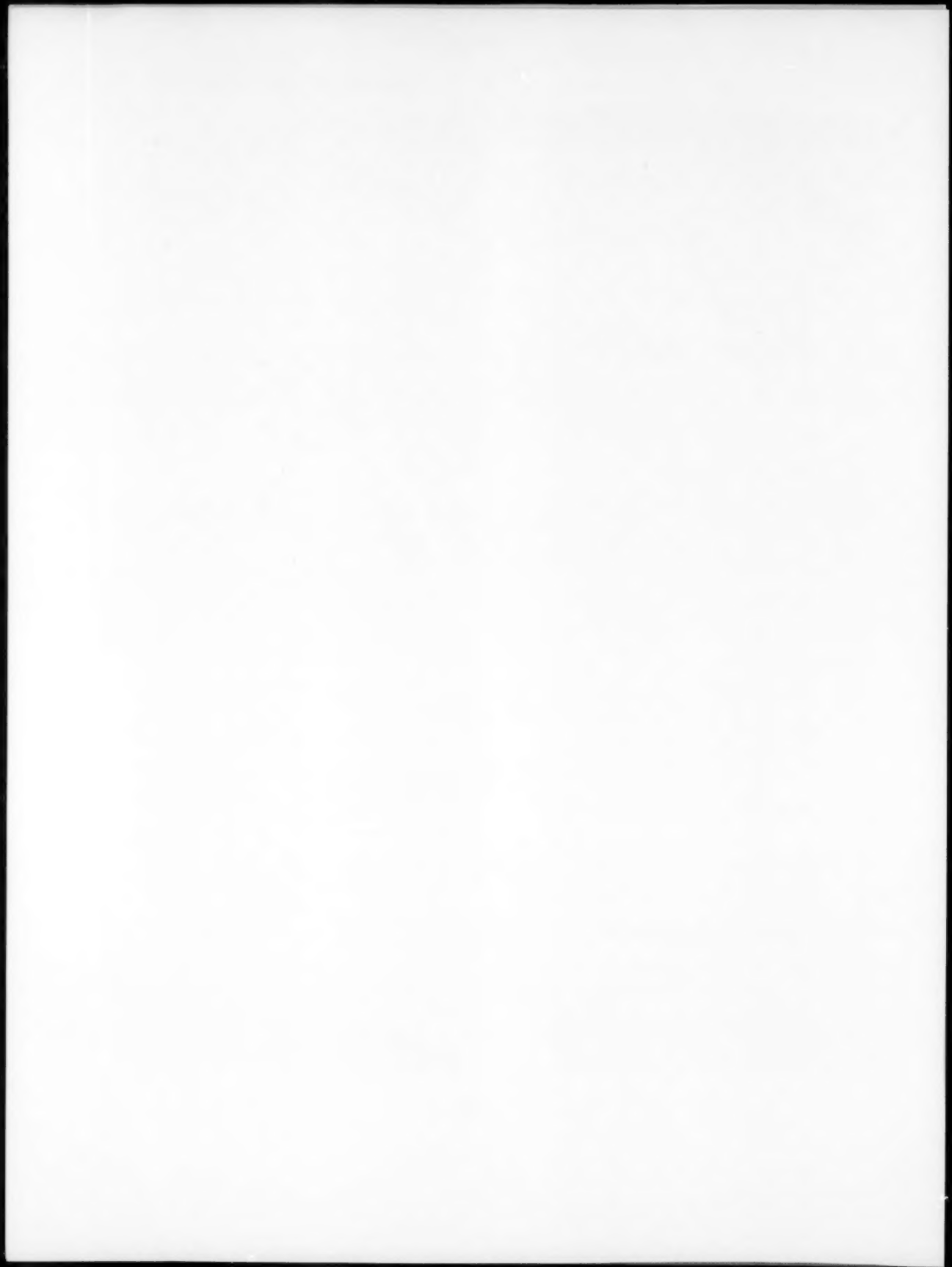
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JOURNAL OF THE CHEMICAL SOCIETY

The scale and cost of present day publication make it necessary to ask authors to co-operate with the Society to the full. To facilitate this the Society will publish a sequence of notices to authors within these covers. It is intended to deal with all major aspects of the

preparation, submission, content, and handling of articles intended for the *Journal*. Careful attention to these notices will help authors to have their work published more easily and rapidly.

NOTICES TO AUTHORS—No. 1

General Policy

The *Journal of the Chemical Society* is a medium for reporting selected original and significant contributions to new chemical knowledge. Articles which do not advance knowledge (e.g. reviews) will not normally be considered for publication in the *Journal*.

All contributions are judged on the criteria of (i) originality and quality of scientific content and (ii) appropriateness of the length to content of new science. Thus, papers reporting results which would be routinely predicted or result from application of standard procedures or techniques are unlikely to prove acceptable in the absence of other attributes which themselves make publication desirable.

Although short articles are acceptable, the Society strongly discourages fragmentation of a substantial body of work into a number of short publications. Unnecessary fragmentation will be a valid reason for rejection of manuscripts.

The *Journal* is published in five Transactions: Dalton, Inorganic; Perkin I, Organic and Bio-organic; Perkin II, Physical Organic; Faraday I, Physical; Faraday II, Chemical Physics.

Authors are requested to indicate, at the time they submit a typescript, the Transactions for which it is intended. Should this seem unsuitable, the Editor will inform the author.

Conditions Governing Acceptance

Contributions which have appeared or have been accepted for publication with essentially the same content in another journal or which incorporate freely available printed work will not be published in the *Journal* except by permission of the Council. This restriction does not apply to results previously published in materially abbreviated form, as a paper presented at a symposium, as a communication to

Chemical Communications, as a letter to the Editor of other periodicals, or as a patent.

Contributions are accepted by the Society on the understanding that the authors (a) have obtained any necessary authority for publication, and (b) will, if requested, surrender their copyright to the Society.

Authors are solely responsible for the factual accuracy of their contributions.

Since the Society reserves the right to retain all typescripts sent to it, authors are advised to keep copies. When contributions have been submitted for publication the authors are not at liberty, save by permission of the Society, to withdraw or delay them or to publish them elsewhere until after publication by the Society.*

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Typescripts should be addressed to: The Manager Journals, The Chemical Society, Burlington House, London W1V 0BN.

Three copies of the typescript (a top copy and two good quality carbon or Xerox copies) are required.

Rapid publication is aided by careful preparation of text and illustrations and strict adherence to the format and conventions of individual Transactions; detailed Instructions to Authors are available on request from the Editor.

Particular attention is drawn to the use of (i) SI units and associated conventions, (ii) I.U.P.A.C. nomenclature for compounds, and (iii) standard methods of literature citation.

Administration

Receipt of a contribution for consideration will be acknowledged immediately by the Editorial Office. The acknowledgement will indicate the paper reference number assigned to the contribution. Authors are particularly asked to quote it on all subsequent correspondence.

* Attention is drawn to the following extract from the Society's Bye-Laws:

84. (i) Every Fellow who, with a view to its publication by the Society, submits a paper or other communication shall by so doing undertake:

(a) that his communication has not been published and that he will not permit its publication before it is accepted or declined by the Society, and

(b) that if it is accepted for publication the Society shall thereupon become entitled to the copyright therein and that he will, when called on to do so, assign, insofar as he is permitted to do so, to the Society the said copyright, including the sole right to print and publish in any form, in any language, and in any part of the world, the whole or any part of his communication. The Council shall not refuse any reasonable request from any author to reproduce his own work elsewhere in whole or in part.

The attention of every Fellow who submits a paper or other communication for publication shall be drawn to this Bye-Law.

(ii) Any person other than a Fellow who submits any paper or other communication with a view to its publication shall be required to sign an undertaking in the terms set out above.

Presentation of Papers

Every latitude, consistent with brevity, in the form and style of papers is permitted, and no pattern for either is prescribed. Certain elements are, however, common to all papers, and these are considered.

Organization of Material

Title.—The choice of a title for a paper is of the greatest importance, since it is from the title that the important key-words used in information retrieval are taken. Not only should the title clearly and accurately indicate the content of that paper but also it should be as specific as the content and emphasis of the work permits. Brevity in a title, though desirable, should be balanced against its accuracy and usefulness.

Abbreviations, symbols, and formulae are generally not permitted, and it is usual to spell out terms where necessary.

Reference to the preceding part of a series must be made as the reference (numbered I) to the title in the form: 'The Chemistry of Vitamin B₁₂. Part VIII.¹ Controlled Potential Reduction of Vitamin B_{12a}.' [Reference to a preceding part in the references is in the form: Part VII, H. A. O. Hill, B. E. Mann, J. M. Pratt, and R. J. P. Williams, *J. Chem. Soc. (A)*, 1968, 564. If the page number is unknown because the paper has still to be accepted, or is in the press, the paper number should be given.]

Summary.—Every paper for the *Journal* must be accompanied by a summary (50–250 words) setting out briefly and clearly the objects and results of the work. The summary should give a reader a clear idea of what the work has achieved and should be *independent* of the main text. This last point is of particular importance in connection with the names of compounds which, although they may be accompanied by a number which refers to a displayed formula in the body of the text, must be comprehensible without reference to this formula. Thus,

Apetalactone, a new triterpene lactone isolated from *Calophyllum apetalum* Willd. has been shown to be 4,28-dihydroxy-3,4-secofriedelan-3-oic acid lactone (IIa).

or

Reaction of sodium hydride with ω -hydroxyalkyl-triphenylphosphonium salts $\text{Ph}_3\text{P}^+[\text{CH}_2]_n\text{OH X}^-$ (I) has been investigated. The salt (I; $n = 1$, $\text{X} = \text{I}$) gave triphenylphosphine and formaldehyde. The salt (I; $n = 2$, $\text{X} = \text{I}$) gave triphenylphosphine oxide and ethylene. Similar reactions were carried out with ω -hydroxyalkyltriphenylarsonium (XIV) and ω -hydroxyalkyldimethylphenylammonium (XV) salts.

The summary should concern only the main subject of the work and its main conclusions; details of an involved argument or synthesis should not be included and, although classes of compounds prepared or discussed should be given rather than a list of compounds, key compounds in the work should be referred to.

Introduction.—This should give clearly and briefly, with relevant references, both the nature of the problem under investigation and its background.

Results and Discussion.—It is usual for the results to be presented first, and for them to be followed by a

discussion of their significance. Only relevant results should be presented, and figures, tables, and equations should be used only for purposes of clarity and brevity. Data must not be reproduced in more than one form, e.g. in both figures and tables.

Experimental Section.—Descriptions of experiments should be given in detail sufficient to enable experienced experimental workers to repeat them; the degree of purity of materials should be given, as should the relative quantities used. Descriptions of established procedures are unnecessary. Standard techniques and methods used throughout the work should be stated at the beginning of the section. Apparatus should be described only if it is non-standard; commercially available instruments are referred to by their stock numbers (e.g. Perkin-Elmer 137 or Unicam SP 500 spectrophotometers). The accuracy of primary measurements should be stated. Unexpected hazards encountered during the experimental work should be noted. The detailed treatment of the Experimental section is dealt with in a forthcoming Notice to Authors.

Acknowledgements.—Contributors, other than co-authors, are acknowledged in a separate paragraph at the end of the paper; acknowledgements should be as brief as possible. Titles, Mr., Mrs., Miss, Dr., Professor, etc., are given; degrees are not given. Organizations which operate on a commercial basis are not acknowledged.

Bibliographic References.—These are given on a separate sheet at the end of the manuscript and are referred to in the text by superior roman numerals. They must be distinguished from footnotes which are given at the bottom of the page to which they refer; they are referred to by an asterisk (*), dagger (†), etc. Bibliographic references and footnotes are the subject of Notice No. 3.

General Detail

Type Size.—It should be noted that since the Experimental section and the results are printed in smaller type than the theoretical part, division between the two should be clear-cut and frequent alternation is not advisable.

Brevity.—Because of the large volume of work submitted for publication, brevity in the presentation of papers is essential and, for this reason, certain tendencies are discouraged; these are as follows:

- Unnecessary division of work into separate parts of a series. Papers are in no way discouraged solely on grounds of length.
- Submission of fragmentary work when this can be included in a larger communication.
- Historical introductory paragraphs in cases when a simple statement of the accepted present position suffices.
- Undue elaboration of hypotheses.
- Over-detailed and verbose exposition of ideas.
- Excessive use of diagrams, for example, straight-line plots that can be adequately expressed as an equation together with, if necessary, a table of deviations.
- Duplication of data as between text, tables, and figures, etc.

(h) Details of the preparation of simple derivatives such as esters, ethers, semicarbazones, *etc.*, and slight variations of essentially the same technique. (Unless the conditions are critical, quantities are superfluous, and only an indication of reagents and/or conditions is required.)

Spelling.—Standard English spelling is used (*Oxford English Dictionary*), although latitude with respect to alternative spellings for certain words is allowed. Where one form or the other of a particular spelling is adopted it should be used consistently throughout a paper.

Punctuation.—Although punctuation follows standard English practice, the following conventions are observed:

- A comma is placed before 'and' or 'or' in a series such as 'oxygen, sulphur, and selenium' or ' λ_{max} 237, 295, and 343 nm.'
- Parentheses, square brackets, and braces are used, as necessary, in that order, *i.e.* {[()]}.
- When a word is followed by a punctuation mark the parenthetical phrase must be inserted before the latter, *e.g.* 'm.p. 234° (decomp.)' and not 'm.p. 234°, (decomp.)'.
- A colon is used to separate a ratio, as in 1 : 20—not a solidus 1/20.
- Parenthetical expressions of the same physical quantity in different units are separated by a comma (3.9 g, 0.1 mol) (30 ml, 1 mol); expressions of different physical quantities are separated by a semicolon (2.9 N; 30 ml) (d 0.88; 8 ml).

Hyphenation.—Hyphens are used for two purposes: to divide and to compound.

Division. It is common practice to divide words, particularly when in a sequence, when one part is common to several of the words; in such cases, the hyphen, representing the point of attachment to the common part, is always inserted, *e.g.* 'the chloro-, bromo-, and fluoro-naphthalenes,' 'the *o*-, *m*-, or *p*-nitrotoluenes,' or 'the oxo-naphthalenes and -naphthalenes.' It is not good practice, however, to detach both a common prefix and a common suffix in a series, *e.g.* 'the dihydroxy- naphthalene- and phenanthrene-diones,' since confusion can arise.

'Sections' of class names such as diazo-ketone, alkyl-diamine, epoxy-nitro-sulphone, *etc.*, are linked by hyphens.

It is also Society usage to insert a hyphen after a prefix which ends in a vowel or y; the hydroxy-group, the aza-function, the carboxy-compounds, the nitro-derivatives, but the methyl group (note that hydroxy, acetoxy, carboxy, ethoxy, and methoxy are used and not hydroxyl, acetoxyl, carboxyl, ethoxyl, and methoxyl).

It is customary to separate a pair of the same letter when these letters (in the same font) would not naturally fall together, *e.g.* butyl-lithium, iodo-octane.

Compounding. A hyphen is often necessary when words are compounded to form a single modifying adjective to precede the noun being modified, thus: 'a melting-point determination' or 'a free-radical chain mechanism.' A hyphen is not needed when adverbs are compounded, as in 'an electrically heated oven,' or for two-word chemical names such as 'nitric acid solution.'

Miscellaneous uses of hyphens. Hyphens are used to set apart numbers, configurational letters, Greek

letters, and italicized prefixes: 1,2,5-trimethylcyclohexane, *D*-gluco-hexose, *s*-trinitrobenzene, β -chlorophenethylbenzene, tri- μ -carbonyl-bis(tricarbonyliron), and 3-methylpent-*trans*-2-ene.

Use of Italics.—As described below, italics are indicated in a typescript by single underlining. Particular attention should be paid to the following uses.

(a) Foreign words and phrases and Latin abbreviations are given in italics: *e.g.*, *in toto*, *in vivo*, *ca.*, *cf.*, *i.e.*, *etc.*

(b) In the names of chemical compounds or radicals italics are used for prefixes (other than numerals or symbols) when they define the position of named substituents, or when they define stereoisomers: other prefixes are printed in roman. (Note: Initial capital letters are not to be used with italic prefixes or single-letter prefixes: full points are not to be associated with letter prefixes.)

o-, *m*-, and *p*-nitrotoluenes, but *ortho*-, *meta*-, and *para*-compounds (*o*-, *m*-, and *p*- are used only with specific names; *ortho*-, *meta*-, and *para*- are used with classes), *s*-trinitrobenzene, *NN*-dimethylaniline, *trans*- and *cis*-hexane-1,2-diol, *gem*- and *vic*-diols, benzil *anti*-oxime, 3-*O*-methyl-L-glycero-tetrolucose.

At the beginning of a sentence the first roman letter after the prefix is capitalized: '*D*-glycero-*D*-gluco-Heptose was subjected . . . ' and ' *β* -*p*-Tolylchalcone gave . . . '

(c) The scientific names of genera, species, and varieties are italicized.

(d) In references to periodicals their names or abbreviations are set in italics.

Note: Greek letters are not italicized, and should not therefore be underlined in typescripts.

Headings.—(a) Main sections (Experimental, Discussion, *etc.*): side-heading, small capitals, no final fullstop.

(b) Main side-heading: italics, initial capital letter for each noun and adjective, final fullstop and dash.

(c) Subsidiary side-heading: italics, first initial capital only, final fullstop but no dash.

(d) Further subdivision: by italic (a), (b), *etc.* (no following fullstop), and finally (i), (ii), *etc.* If (a), (b), *etc.* are used in front of a subsidiary side-heading, then for contrast these letters are not italicized.

Letters and prefixes which are ordinarily printed in italics are transferred for contrast into roman type in italicized phrases (see example below, where *O*-alkyl becomes *O*-alkyl).

Physicochemical symbols, however, remain in their prescribed form, and numerals and Greek letters are not italicized.

Examples:

EXPERIMENTAL

Preparation of Aliphatic Aldoximes and Ketoximes.

—Acetoxime *O*-alkyl ethers. (a) Acetoxime (100 g) was dissolved . . .

Density (*d*) of the Alcohol at 295 K.—The series of aliphatic alcohols . . .

Note: In the above examples it should be noted that the type of print required to indicate italics, capitals, small capitals, *etc.* is shown by underlining; this convention must be strictly adhered to, *i.e.*

Single underlining for italic type

Double underlining for SMALL CAPITALS

Treble underlining for ORDINARY CAPITALS

Wavy underlining for bold black type

NOTICES TO AUTHORS—No. 3/1968

Bibliographic References and Footnotes

A clear distinction is made between bibliographic references and footnotes. The latter are used to present material which, if included in the body of the text, would disrupt the flow of the argument but which is, nevertheless, of importance in qualifying or amplifying the textual material. Such footnotes are referred to with the following symbols: *, †, ‡, §, ¶, ||, etc. [Note: Since an asterisk is used to indicate the author to whom correspondence should be addressed, its use early on in a paper is not advised; a dagger (†) is preferred.]

Bibliographic References.—Reference to the source of statements in the text is made by use of *superior numerals* at the appropriate place. The references themselves are given as footnotes at the bottom of the corresponding page in the final printed text. It is thus *essential* that bibliographic references are numbered in the order in which they will appear.

When citation of a paper is repeated the numeral previously given to that reference is to be used also at the second citation; the footnote is not repeated.

The position of the superior numeral should be chosen with care, particularly when it does not follow an author's name. If placed adjacent to punctuation, the numeral should normally be placed after the punctuation mark, e.g. 'This compound was shown to be the dienone,³ which...'. It may be necessary to modify this rule, however, to avoid confusion, thus: 'In this way the method was found to be suitable for lead², tin³, bismuth⁴, and mercury⁵.'

Particular care is necessary where a reference number is likely to be confused with a superscript numeral indicating a power index: '... which gave a value of 2.3 cm³...' should be written as '... which gave a value³ of 2.3 cm' or '... which gave a value of 2.3 cm (ref. 3)'.

Since it is usually difficult to print a table in a given position in the text, references within the table are best dealt with by taking the individual references into the printed footnotes to the tables and using a new reference number sequence therein. Should the references cited in the tables appear much earlier in the text, these earlier reference numbers may be used.

Journals. New instructions for the abbreviation of journal titles will be issued early in 1980. At the present time where authors have difficulty in deciding on a suitable journal abbreviation they are invited either to write directly to the Editors or to consult current copies of the *Journal*.

Books. Titles of books are cited in quotation marks, in upright letters, and the author(s), title, publisher, town, date (or edition, if more than one has

been published), and page number (if required) must be given in that order:

C. J. M. Stirling, 'Radicals in Organic Chemistry,' Oldbourne Press, London, 1965, p. 69.

T. J. Suen, in 'Polymer Processes,' ed. C. E. Schildknecht, Interscience, New York, 1956, vol. X, p. 295.

Patents. Patents should be indicated in the form: B.P. 367,450, 367,455-7. U.S.P. 1,171,230. G.P. 436,112-4. Jap.P. 20,101. Dates are indicated thus: B.P. 666,776/1956. Patents which are applied for must always be given a year, e.g. B.P. Appl. 102/1968.

Reports and Bulletins, etc.

R. A. Allen, D. B. Smith, and J. E. Hiscott, 'Radioisotope Data,' UKAEA Research Group Report AERE-R 2938, H.M.S.O., London, 1961.

'Collected Papers on Methods of Analysis for Uranium and Thorium,' Geological Survey Bulletin 1006, U.S. Government Printing Office, Washington D.C., 1954.

Material presented at meetings.

N. N. Greenwood, Abstracts, Anniversary Meeting of the Chemical Society, Glasgow, 1965, C1.

N. S. Anderson and D. A. Rees, in 'Proceedings of the Vth International Seaweed Symposium,' ed. E. G. Young and J. L. McLachlan, Pergamon Press, Oxford, 1966, p. 405.

Theses.

A. D. Mount, Ph.D. Thesis, University of London, 1967.

Reference to unpublished material. For material presented at a meeting, congress, or before a society, etc., but not published, the following form is used:

¹ A. R. Jones, presented in part at the XXth Congress of the International Union of Chemistry, Paris, September, 1960.

For material accepted for publication, but not yet published, the following form is used:

² A. R. Jones, *J. Amer. Chem. Soc.*, in the press.

If the paper has been submitted to the Society, the paper number should be given:

³ A. R. Jones, *J. Chem. Soc. (A)*, in the press (8/556).

For material submitted for publication but not yet accepted the following form is used:

⁴ A. R. Jones, submitted for publication in *Angew. Chem.*

For personal communications the following form is used:

⁵ G. B. Ball, personal communication. (Note: the form, G. B. Ball, private communication, is inappropriate.)

If material is to be published but has yet to be submitted the following form is used:

⁶ Unpublished data.

Names.—The names and initials of all authors are always given in the reference footnote; they must not be replaced by the phrase *et al.* This does not prevent some, or all, of the names being mentioned at their first citation in the cursive text: initials are not necessary in the text.

For Chinese and Spanish authors all names should be given as in the original, since the patronymic is not always given last in these languages. If co-authors are to be collectively cited, as in 'Smith and his co-workers' or 'Smith *et al.*,' the latter form is inappropriate unless the individual name 'Smith' appears first among the authors named in the original.

Composite References.—Whenever possible, composite references should be used rather than a series of individual references. The style for composite references is as follows:

¹ A. B. Jones, *J. Chem. Soc. (A)*, 1967, 234.

² A. B. Jones, *J. Chem. Soc. (A)*, 1966, 123; 1967, 234.

³ A. B. Jones, *J. Chem. Soc. (A)*, 1966, 123; *J. Amer. Chem. Soc.*, 1956, 78, 1234.

⁴ A. B. Jones, *J. Chem. Soc.*, 1956, 234; A. B. Jones and C. D. Brown, *J. Chem. Soc. (B)*, 1967, 234, 1077; 1968, 599.

⁵ A. B. Jones, *J. Amer. Chem. Soc.*, 1956, 78, 1234; A. B. Jones and C. D. Brown, *ibid.*, 1957, 79, 567; A. B. Jones and E. F. Green, *ibid.*, p. 999.

If only one paper from a composite reference is required for citation later, then two numbers may be assigned to the first citation (e.g. Jones ^{1,2}); alternatively, long composite references may be divided by letters, e.g.:

(a) A. B. Jones, *J. Chem. Soc. (A)*, 1954, 467;

(b) A. B. Jones and C. D. Brown, *J. Chem. Soc. (B)*, 1967, 234.

A. B. Jones, *J. Chem. Soc. (A)*, (a) 1953, 267;

(b) 1954, 1742; (c) *etc.*

A composite reference may cite a previous reference in the form:

¹² A. B. Jones, *J. Chem. Soc.*, 1956, 234; C. D. Brown, *ref. 5*.

(Note: *ibid.* is used only within a given reference and not to refer from one reference number to another: the abbreviated title for the journal should be repeated for separate reference numbers.)

Idem, *loc. cit.*, and *op. cit.* are not used in references.

NOTICES TO AUTHORS—No. 5/1969

The International System of Units (SI)

Preamble

For many years the practice of The Society in respect of units has been based on the recommendations of a joint Committee of The Royal Society, The Chemical Society, The Faraday Society, and The Physical Society. The 1951 set of recommendations published by that Committee formed the basis of Chapter 7 of the 'Handbook for Chemical Society Authors' but since their promulgation much effort has been expended in international circles to devise and approve a basic set of coherent units. This having been completed, The Joint Symbols Committee of The Royal Society, of which The Chemical Society is a participating member, has produced a completely new set of recommendations in a pamphlet 'Symbols, Signs and Abbreviations' 1969 (copies of this pamphlet or further details can be obtained from the Managing Editor, The Chemical Society, Burlington House, London, W1V 0BN). The basis of the new recommendations is the 'Système International d'Unités' (to be abbreviated to SI, in all languages).

The advantages offered by SI are as follows.

- (i) It is a truly coherent system, *i.e.* the product or quotient of any two unit quantities in the system is the unit of the resultant quantity. This contrasts with the previous situation where, even in metric systems used within the same discipline, many additional units are arbitrarily and sometimes differently defined.
- (ii) SI derives nearly all the quantities needed in all sciences and technologies from a very small set of base-units.
- (iii) The variety of multiples and sub-multiples in common use is minimized.
- (iv) A more uniform presentation can be ensured.
- (v) Presentation is such that the relation of any derived unit, or multiple or sub-multiple of a derived unit, to the coherent unit is always obvious and simple.

Policy

(1) The Society announces its approval and support of SI, and its intention that SI shall become the preferred system in its publications.

(2) *Guidelines for the publications of the Society.* The Society realises that public acceptance of this system will be more a matter of education and tolerance than of dictatorial action. It nevertheless desires that the SI system and units compatible with it shall rapidly become the established standard in the Society's publications. An author will not be denied any reasonable usage, but if non-SI units are used for critical data or for quantities measured to a high order of accuracy (as opposed to the rough physical conditions of an experiment), the definitive values will be expressed in SI units as well.

The following will be the guidelines used:

- (a) A metric system will always be used in preference to a non-metric one.
- (b) The SI system will be the standard usage.

- (c) The units used to record the *definitive* values of 'critical data' or quantities measured to high degree of accuracy will be of the SI system.
- (d) When non-SI units are used they must be adequately explained unless their definition is obvious (*e.g.* degree Celsius, mmHg, g, h). The derivation of derived non-SI units will be indicated.
- (e) Equations involving electrical quantities should normally be those appropriate for use with SI (rationalized m.k.s) units. If authors wish to use equations suitable for e.s.u. or e.m.u. the lack of consistency with SI units must be explicitly noted.
- (3) *The principal changes.* There are four of these:
 - (a) Basic units: the metre and the kilogramme replace the centimetre and the gramme of the old metric system.
 - (b) The unit of force is now the newton (kg m s^{-2}).
 - (c) The unit of energy is the joule and of power the joule per second (watt); thus the variously defined calories and non-metric units of energy and power are superseded.
 - (d) 'Electrostatic' and electromagnetic units are replaced by SI electrical units.

Detail

(4) *Definition.* A quantity is expressed as the product of a numerical value and a unit.

(5) *The System.* The fully coherent SI consists of base-units, supplementary units, derived units, and decimal multiples and sub-multiples of these units, formed by use of prefixes only.

(6) *Coherent systems.* A coherent system is one based on a selected set of 'base-units' from which 'derived units' are obtained by multiplication without introducing numerical factors.

(7) *Base-units.* The name International System of Units (SI) was adopted by the Conférence Générale de Poids et Mesures in 1960 for the coherent system now based on the base-units given in Table 1.

TABLE 1		
Physical quantity	Name of base-unit	Symbol for unit
length	metre	m
mass	kilogramme	kg
time	second	s
electrical current	ampere	A
thermodynamic temperature	kelvin	K
luminous intensity	candela	cd
amount of substance	mole	mol

(8) *Supplementary units.* The SI also includes two 'supplementary' dimensionless units as follows:

Physical quantity	Name of unit	Symbol for unit
plane angle	radian	rad
solid angle	steradian	sr

(9) *Multiples and sub-multiples.* In the SI there is one and only one basic unit for each physical quantity. Decimal fractions and multiples of these basic units may, however, be constructed by use of certain prefixes (see Table 2). They may also be used with derived SI units.

TABLE 2					
Fraction	Prefix	Symbol	Multiple	Prefix	Symbol
10 ⁻¹	deci	d	10	deka	da
10 ⁻²	centi	c	10 ²	hecto	h
10 ⁻³	milli	m	10 ³	kilo	k
10 ⁻⁶	micro	μ	10 ⁶	mega	M
10 ⁻⁹	nano	n	10 ⁹	giga	G
10 ⁻¹²	pico	p	10 ¹²	tera	T
10 ⁻¹⁵	femto	f			
10 ⁻¹⁸	atto	a			

The combination of a prefix and a unit symbol constitutes a new single unit symbol; compounding of prefixes is not permitted.

Although it will not always be possible, particularly in Tables, the general principle should be to choose a unit (*i.e.* including multiple or sub-multiple) such that the resulting numerical value is between 0.1 and 1000.

(10) *Derived units.* Some derived units have special names and symbols, and these are given in Table 3.

TABLE 3				
Physical quantity	Name of SI unit	Symbol for SI unit	Definition of SI unit	
energy	joule	J	kg m ² s ⁻²	
force	newton	N	kg m s ⁻² = J m ⁻¹	
power	watt	W	kg m ² s ⁻³ = J s ⁻¹	
electric charge	coulomb	C	A s	
electric potential difference	volt	V	kg m ² s ⁻³ A ⁻¹ = J A ⁻¹ s ⁻¹	
electric resistance	ohm	Ω	kg m ² s ⁻³ A ⁻² = V A ⁻¹	
electric capacitance	farad	F	A ² s ⁴ kg ⁻¹ m ⁻² = A s V ⁻¹	
magnetic flux	weber	Wb	kg m ² s ⁻² A ⁻¹ = V s	
inductance	henry	H	kg m ² s ⁻² A ⁻² = V A ⁻¹ s	
magnetic flux density	tesla	T	kg s ⁻² A ⁻¹ = V s m ⁻²	
luminous flux	lumen	lm	cd sr	
illumination	lux	lx	cd sr m ⁻²	
frequency	hertz	Hz	s ⁻¹	

Others do not

Physical quantity	SI unit	Symbol for SI unit
area	square metre	m ²
volume	cubic metre	m ³
density	kilogramme per cubic metre	kg m ⁻³
velocity	metre per second	m s ⁻¹
angular velocity	radian per second	rad s ⁻¹
acceleration	metre per second squared	m s ⁻²
pressure	newton per square metre	N m ⁻²
kinematic viscosity, diffusion coefficient	square metre per second	m ² s ⁻¹
dynamic viscosity	newton second per square metre	N s m ⁻²
electric field strength	volt per metre	V m ⁻¹
magnetic field strength	ampere per metre	A m ⁻¹
luminance	candela per square metre	cd m ⁻²

(11) *Symbol.* The symbol for a unit will be printed in roman (upright) type, remains unaltered in the plural and does not take a full point, *i.e.* 5 cm not 5 cm. or 5 cms or 5 cms.

The symbol will be separated from the numerical value by a thin space.

(12) *Decimal fractions and multiples of SI units having special names.* These names are not part of the SI, but for the time being their use in The Society's publications may continue. The list given in Table 4 is not exhaustive.

TABLE 4			
Physical quantity	Name of unit	Symbol unit	Definition of unit
length	ångström	Å	10 ⁻¹⁰ m = 10 ⁻¹ nm
length	micron	μm	10 ⁻⁶ m
area	barn	b	10 ⁻²⁸ m ²
volume	litre	l	10 ⁻³ m ³ = dm ³
mass	tonne	t	10 ³ kg = Mg
force	dyne	dyn	10 ⁻⁵ N
pressure	bar	bar	10 ⁵ N m ⁻²
pressure	pascal	Pa	N m ⁻²
energy	erg	erg	10 ⁻⁷ J
kinematic viscosity			
diffusion coefficient	stokes	St	10 ⁻⁴ m ² s ⁻¹
dynamic viscosity	poise	P	10 ⁻¹ kg m ⁻¹ s ⁻¹
magnetic flux	maxwell	Mx	10 ⁻⁸ Wb
magnetic flux density			
(magnetic induction)	gauss	G	10 ⁻⁴ T
conductance	siemens	S	Ω ⁻¹

(13) *Units defined in terms of the best available experimental values of certain physical constants.* These units are not part of the SI. The factors for conversion of these units to SI units are subject to change in the light of new experimental measurements of the constants involved. Their use outside the restricted contexts to which they are appropriate should be discouraged. The following list is not exhaustive.

Physical quantity	Name of unit	Symbol for unit	Conversion factor
energy	electronvolt	eV	eV ≈ 1.6021 × 10 ⁻¹⁹ J
mass	unified atomic mass unit	u	u ≈ 1.66041 × 10 ⁻²⁷ kg

(14) *Other units now exactly defined in terms of the SI units.* These units are not part of the SI. It is recognized that their use may be continued for some time but it is recommended that except in special circumstances they should be progressively abandoned in conformity with international recommendations. The list given in Table 5 is by no means exhaustive. Each of the definitions given in the fourth column is exact.

TABLE 5			
Physical quantity	Name of unit	Symbol for unit	Definition of unit
length	inch	in	2.54 × 10 ⁻² m
mass	pound (avoirdupois)	lb	0.453 592 37 kg
time *	minute	min	60 s
time *	hour	h	3600 s
force	kilogramme-force	kgf	9.806 65 N
force	pound-force	lbf	9.806 65 × 0.453 592 37 N
pressure	atmosphere	atm	101 325 N m ⁻²
pressure	conventional millimetre of mercury	mmHg	13.5951 × 9.806 65 N m ⁻²
pressure	torr	Torr	(101 325/760) N m ⁻²
pressure	pound-force per square inch	lbf in ⁻²	$\frac{9.806\ 65 \times 4535.9237}{6.4516}$ N m ⁻²
energy	kilowatt hour	kW h	3.6 × 10 ⁶ J
energy	thermochemical calorie	cal(thermochem.)	4.184 J
energy	I.T. calorie	cal _{I.T.}	4.1868 J
thermodynamic temperature	degree Rankine	°R	(5/9) K
radioactivity	curie	Ci	3.7 × 10 ¹⁰ s ⁻¹

* Use of other common units (min, h, day) may continue in normal expressions of intervals of time.

Formulae and Figures

The purpose of all illustrative matter in a paper is to clarify the arguments and descriptions rather than to duplicate them. The Society strongly encourages the use of displayed formulae, particularly in the form of schemes where the details of a reaction sequence are often more easily understood when illustrated than when described in the text.

All formulae and figures should be clearly drawn, and in the case of figures provided with captions; the latter should be typed on a separate sheet. Since all formulae carry a key number by which they are identified, unless they form part of the running text or unless they are part of a scheme which itself has a caption, they are not generally further described. Blocks of formulae do not need a caption.

Illustrative matter is divided, for technical reasons, into figures and formulae, although in many cases (e.g. crystal structures which may be regarded as formulae but which are treated as figures) these divisions overlap.

Structural Formulae.—(a) Only those formulae which are displayed may be given key numbers. In all other cases the compounds concerned are referred to by name only.

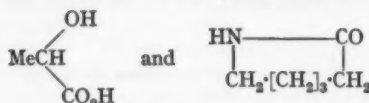
(b) Formulae are numbered sequentially with bold arabic numerals in parentheses [(1), (2), and (3) *etc.*] as they are displayed and *not* as they are mentioned in the text.

(c) In complex reaction schemes the formulae should be numbered serially following the reaction sequence. Non-sequential numbering in a collection of formulae can render it hard to locate an individual number.

(d) Structural or displayed formulae must be carefully and accurately drawn or typed on a separate sheet, rather than inserted into the text, although a marginal indication of where they are to go in the text is desirable.

(e) Formulae inserted into the body of the text (as distinct from those displayed separately) should be written on one line if possible, e.g.

$\text{HO}\cdot\text{CHMe}\cdot\text{CO}_2\text{H}$ and $\text{NH}\cdot[\text{CH}_2]_5\cdot\text{CO}$ rather than



(f) Points (which may be typed as full stops) are used to indicate bonds between the atoms of the backbone chain of a compound. The symbol of each element of that chain is preceded by a full stop (or colon for a double bond) and followed by the symbols or formulae of the atoms or groups that are attached to it (parentheses being used where necessary to enclose compound groups), e.g. $o\text{-HO}\cdot\text{C}_6\text{H}_4\cdot\text{CH}_2\cdot\text{NH}_2$ and $\text{CH}_2\text{Cl}\cdot\text{CH}(\text{OH})\cdot\text{CO}_2\text{H}$.

Groups that are indicated by a single symbol (e.g. Me and Et *etc.*) do not need use of such full stops.

Repeating sequences of a backbone composite group are enclosed with square brackets and their number is indicated by an inferior multiplier, e.g. $\text{HO}\cdot[\text{CH}_2]_4\cdot\text{NH}_2$, but $\text{HO}\cdot[\text{CH}_2]_4\cdot\text{N}(\text{CH}_2\text{-OH})_2$.

(g) The use of large circles to represent six delocalized π -electrons in cyclic systems (with or without positive or negative signs as appropriate) is permitted in certain circumstances. Cyclic systems with more or less than six delocalized π -electrons may be represented by formulae containing dotted lines. Both topics are dealt with in *Proceedings*, 1959, 75.

(h) Customary steric conventions must be observed, notably for steroids, triterpenes, and carbohydrates. The Society uses wedges (\blacktriangle) or heavy lines (—) rather than blocked circles (\bullet) and broken lines in the form ----- rather than ||||| .

(i) The symbols Me, Et, Prⁿ, Prⁱ, Buⁿ, Buⁱ, Bu^s, Bu^t, Ph, Ac, Bz (the symbol for PhCO and not for PhCH₂), Alk, Ar, and Hal, should be used but may be written in full when the groups are involved in the reaction described. Other special symbols, if used, require an explanatory footnote. The carboxy-group is written CO₂H (*not* COOH) and similarly CO₂R.

(j) One variable univalent substituent is indicated by R; when more than one independently variable general substituent is present, R¹, R², and R³ should be used (*not* R, R¹, R², R³; or R₁, R₂, and R₃ which indicate $1 \times R$ and multiples of R thereof).

(k) Often it is desirable to use one formula to represent a number of related compounds (or classes of compounds) by the use of one or more independently variable substituents. It is preferable to give each compound thus represented a separate key number rather than to subdivide individual key numbers by alphabetical suffixes [*i.e.* (1a), (1b), (1c) *etc.*].



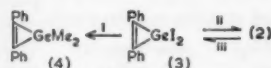
- (1) R¹ = R² = Ph, R³ = Me, X = O
(2) R¹ = Me, R² = R³ = Ph, X = S



- (3) R¹ = Me, R² = Ph, R³ = Bz
(4) R¹R² = CO-O-CO, R³ = Ph

The use of more than four independently variable substituents or atoms on one generalized formula is discouraged.

(1) Once a formula has been displayed it is permissible to employ its key number in later reaction schemes or equations rather than to re-display the formula:



Reagents: i, MeMgI; ii, NaOH; iii, HI

It should be noted that reagents and reaction conditions are given as footnotes to the scheme for economy of space; if present, an equation number is set as far to the right as possible, and if there is likelihood of

confusion with compound key-numbers it is accompanied by the word equation.

(m) Displayed formulae, unless they are capable of being typed on one line [see point (e) above], should not be included in tables; they should be displayed before the table with a key number for each compound and this should be used in the table.

(n) The key number for a compound may be used in the cursive text to avoid repetition of long chemical names; this device must not be used to excess. In general it is preferred if the key number is qualified by a partial name for the compound as in the following example:

'Pyolin (1) was oxidized by permanganate to the oxo-acid (2), the methyl ester (3) of which with methylmagnesium iodide gave the normal product (4)'.

(o) Reference to compounds in the Summary by key number alone is not allowed since a summary should be comprehensible without reference to the body of the paper itself. The reference number should, however, accompany the name of the compound to which it refers.

Figures.—(a) Figures must bear on the back the names of the authors, the title of the paper (abbreviated if necessary), and the number of the figure.

(b) Figures must be in Indian ink, on Bristol board, white smooth cartridge paper, tracing linen, plastic film (it is essential that the special plastic ink developed for this is used), or graph paper with *faint* blue lines (red or brown lines must not be present as these may be reproduced by the photographic process of block making). Since lines must be black and sharp, photostats or similar prints are often not suitable. If paper is used, it must be strong enough to withstand repeated handling.

(c) Lettering and numerals must be in *blue pencil* (not red or black pencil or ink) clearly legible but not so heavily scored as to make a permanent impression on the paper or board.

(d) When the figures are large (more than 8 in \times 10 in), smaller copies (which may be rough, as long as they are clear) should be supplied for submission to the referees; editing will not be undertaken, however, before the final figures are received.

(e) Figures must be carefully drawn, preferably three times the size (linear) that seems necessary to ensure sharp printing, but excessive reduction is costly and illustrations that exceed five times the size of the finished block may be returned to the author for redrawing.

(f) Two-inch margins are essential all round figures. Lettering for insertion at margins should be placed well clear of the ordinate or abscissa line so that it can be copied before erasure.

Lettering and touching-up are done by the Society and clarity of instructions is essential. When there is much lettering, or complicated lettering, and always when tracing linen or plastic film is used, a rough tracing should be added with the lettering shown in ink.

(g) Since, for printing, the size is reduced, lines should not be too thin. Given lines must be of even thickness, angles neat, and curves smooth.

(h) Graphs should have only the requisite minimum of the scale (not less than three points) marked by numerals, and the scale lines should not normally be continued into the body of the figure.

(i) Graphs in any one paper should, when convenient, be drawn to the same scale, and scale markings should, when possible, be identical so that the graphs may be placed adjacent on the page. Contrariwise, two curves drawn to different scales can be shown on one graph by having the appropriate scales on the left-hand and the right-hand side. The use of both right- and left-hand axes and top and bottom axes on figures which have quantitative significance is encouraged.

(j) Experimental points must be shown sufficiently large to be distinguishable when reduced in size. Whenever possible, they should be confined to open and closed circles, crosses, squares, and triangles. Partly black circles and similar signs frequently become indistinguishable in print.

(k) Curves may be distinguished as full lines (—), broken (---) or dotted lines (···), and dot-dash lines (— · — · —); further differentiation should normally be achieved by labelling the curves, which is, in any case, desirable.

(l) For reference in legends, it is preferable to mark curves A, B, C, *etc.* rather than to reproduce the type of line in print.

(m) There must be no unnecessary waste space, *e.g.* around curves; ordinates and abscissae should start at zero only if the curve extends to that range. Enlargement of parts of a figure can occasionally be placed in a corner of the complete figure.

(n) It is not advisable to insert much or complicated lettering on curves or in blank spaces; mistakes (in copying by the artist) can rarely be rectified once the block is made. It is better to label the curves A, B, C, *etc.* and to use explanatory legends.

(o) *Large* solid objects should be represented by hatching rather than by black surfaces, otherwise the ink may smear on printing.

(p) Photographs are reproduced by a half-tone process on art paper. The prints supplied must be very clear and of good contrast, as considerable definition may be lost in reproduction.

(q) Captions and explanatory legends, to be set by the printer should be typed on a separate page attached to the manuscript, and not given on the figure itself.

(r) Figures are numbered consecutively Figure 1, Figure 2, *etc.* (in arabic numerals). Photographs (half-tone reproduction) are numbered consecutively Plate 1, Plate 2, *etc.* but these numbers are independent of the numbering of any figures.

(s) Since figures represent an uneconomical use of space their number and size should be kept to a minimum. Figures and tables for the same values are discouraged.

NOTICES TO AUTHORS—No. 7/1970 (revised 1976)

Deposition of Data—Supplementary Publications Scheme

Preamble

The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are all making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library, Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Chemical Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this 'Supplementary Publications Scheme'.

Bulk information (such as crystallographic structure factor tables, computer programmes and output, evidence for amino-acid sequences, spectra, etc.), which accompanies papers published in future issues of the Chemical Society's *Journal* may in future be deposited, free of charge, with the Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of referees and with the approval of the author.

The Scheme

Under this scheme, authors will submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication the supplementary material will be sent by the Society to the B.L.L.D. where it will be stored. Copies will be obtainable by individuals both in the U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

- (a) Optimum page size for text or tables in type-script: up to 30 cm × 21 cm.
- (b) Limiting page size for text or tables in type-script: 33 cm × 24 cm.
- (c) Limiting size for diagrams, graphs, spectra, etc.:

39 cm × 28.5 cm.

- (d) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.
- (e) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided. If authors have the facilities available the use of a type face designed to be read by computers is encouraged.

Deposition

The Society will be responsible for the deposition of the material with the B.L.L.D. The B.L.L.D. will not receive material direct from authors since the Library wishes to ensure that the material has been properly and adequately refereed.

Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all of this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the B.L.L.D. The Society will add to the paper a footnote indicating what material has been deposited in the Supplementary Publications Scheme, the supplementary publication number, and details as to how copies may be obtained.

Availability

Copies of Supplementary Publications may be obtained from the B.L.L.D. on demand by organizations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

Mr. J. P. Chillag,
British Library Lending Division,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, U.K.

Non-registered users may also obtain copies of Supplementary Publications but should first apply for price quotations. These are available from the Loans Office at the above address.

International Collaboration

A similar scheme (known as the National Auxiliary Publications Service) is being operated in the U.S.A. by the American Society for Information Science. Similar schemes are also being contemplated in other

countries. The provision of reciprocal arrangements for the exchange of supplementary data between the various national deposition centres is being investigated.

NOTICES TO AUTHORS—No. 8/1970

X-Ray Crystallographic Structure Factor Tables

The Society has recently taken advice from the members of its Chemical Crystallography Group and as a result of this and of the inception of the National Lending Library Supplementary Publications Scheme (discussed in Notices to Authors No. 7) the following rules are being taken into use forthwith to govern the publication or deposition of X-ray crystallographic structure factor tables.

(i) The Society will no longer publish tables of structure factors in its publications except in accordance with the provision of paragraph (iv) below.

(ii) All authors of crystallography papers will submit along with the manuscript a readable table of such structure factors for the referees' inspection. The table should be prepared in accordance with the detail given in paragraph 3 of Notices to Authors No. 7 so that it may be used for deposition. Computer print-out may be used providing that it is top copy in good contrast (see note).

(iii) If the referees accept the paper and its associated structure factor tables then the Society will deposit these structure factor tables in the National Lending Library Supplementary Publications Scheme

(see Notices to Authors No. 7) and will publish as a footnote to the paper the necessary details that will enable any reader to obtain a copy in microfiche or an electrophotographic printoff of the data tables associated with the paper.

(iv) Authors, or the referees, may request publication of such tables of structure factors, *in extenso*, in cases that seem to them to be desirable. It is expected that this will occur only rarely.

(v) The details of the National Lending Library Supplementary Publications Scheme and the methods for obtaining photographic printoff of material deposited with that scheme are given in Notices to Authors No. 7.

Note to paragraph (ii). Structure factors tables prepared from computer printout must be presented in the form indicated in paragraph 3 of Notices to Authors No. 7 and must be arranged with the greatest economy of space possible [*i.e.* not less than two groups of columns (h , k , l , F_o , F_o) to the page (30 cm \times 21 cm)]. All columns must be headed. A 'paste-up' on white card of computer printout will be acceptable providing the quality of the printout is adequate.

NOTICE TO AUTHORS—No. 9/1974

Nomenclature

For many years the Society has actively encouraged the use of standard I.U.P.A.C. nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the I.U.P.A.C. rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

In order to encourage authors to use I.U.P.A.C. nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given.

'Nomenclature of Organic Chemistry, Sections A, B, and C,' Butterworths, London, 2nd Edition, 1971.

Nomenclature of Inorganic Chemistry,' Butterworths, London, 1971.

'Manual of Symbols and Terminology for Physicochemical Quantities and Units,' Butterworths, London, 1970.

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids, and steroids, and rules of stereochemistry are available from the:

I.U.P.A.C. Secretariat,
Bank Court Chambers,
2—3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF.

It is recommended that where there are no I.U.P.A.C. rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

NOTICE TO AUTHORS—No. 10/1976

Authentication of New Compounds

(1) It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

(2) In the context of this Notice a compound is considered as new (a) if it has not been prepared before, (b) if it has been prepared before but not adequately purified, (c) if it has been purified but not adequately characterised, (d) if, earlier, it has been assigned an erroneous constitution, or (e) if it is a natural product synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising data; in spite of (c) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.*

(3) Referees are asked to assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compounds, but the Society's policy remains unchanged in that evidence for the unequivocal identification of new compounds should normally include good elemental analytical data; an accurate mass measurement of a molecular

ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Low-resolution mass spectroscopy must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. Where elemental analytical data are not available, appropriate evidence which is convincing to an expert in the field will be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

(4) Spectroscopic information necessary to the assignment of structure should normally be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may always be treated as a Supplementary Publication where their importance does not justify their inclusion in the published paper.

(5) Finally, referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of present standards.

* New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4. $C_{13}H_{12}NO_4$ requires C, 63.2; H, 5.3%). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: 62.95; H, 5.4. Calc. for $C_{13}H_{12}NO_4$: C, 63.2; H, 5.3%). Analyses are normally quoted to the nearest 0.05%.

Publication of X-Ray Crystallographic Work in the *Journal*

Preamble

At a meeting of the Primary Journals Committee held in October 1975 a sub-committee was set up to consider policy with regard to publication in the *Journal* of both preliminary communications and substantive papers concerned with X-ray crystallographic work. This step was taken in the light of correspondence received by the Society which indicated concern by many referees on the problems created by the large number of routine X-ray crystallographic studies submitted to the Society as a result of the increasing ease of carrying out such work.

Since the sub-committee's terms of reference were wide it was able to consider both this problem and others relating to publication of X-ray crystallographic work in all sections of the *Journal*. Its recommendations which are outlined below fall into two groups: those concerned with preliminary communications and those with full papers. These recommendations have been endorsed by the Primary Journals Committee and now represent the Society's policy with regard to crystallographic work submitted for publication in its primary journals.

Preliminary Communications

(1) Evidence was presented to the sub-committee that a major problem associated with the publication of preliminary reports of crystallographic work in *J.C.S. Chem. Comm.* arose as a result of the non-availability to interested readers of the atomic co-ordinates associated with this work. Although in the normal course of events such data would be expected to appear in the follow-up paper, many cases were cited where the period between publication of the preliminary report and the substantive paper was many years or the full papers never appeared in print. The evidence presented suggested that there was considerable disquiet among crystallographers at this state of affairs. In an attempt to improve this situation and after consultation with the Cambridge Crystallographic Data Centre (C.C.D.C.) the Society has resolved to press authors of preliminary reports of X-ray crystallographic work to submit together with their communication certain material for deposition with the Centre.* This material will be checked at the Centre for internal consistency and, afterwards, will be available on request to interested readers. The procedure to be adopted will be as follows:

- (i) In addition to the communication and the customary covering letter of justification the authors will be expected to provide a complete list of refined co-ordinates (in the form of computer print-out and NOT a retyped version) and a table of bond distances unless these are given in full in the manuscript. If the complete 'crystal data' (i.e. cell dimensions and standard deviations, space group, number *Z* of formulae units per cell) are not listed in the manuscript these must also be submitted.

It should be emphasised that the co-ordinates submitted for deposition, whilst not necessarily being 'fully' refined, should correspond to the stage of refinement described in the preliminary communication and should be the set for which the *R* factor is quoted. It follows that all bond distances given in the preliminary communication should correspond, apart from any rounding-off errors, with bond distances which can be calculated from the deposited co-ordinates.

* Applies only to compounds containing organic carbon atoms.

- (ii) The communication will be assessed in the customary fashion, the material for deposition also being made available to the referees concerned. If the communication is accepted the Society will forward the material for deposition to the C.C.D.C. A statement will be made in the communication that particular material is available from the Centre on request.
- (iii) The C.C.D.C. will acknowledge receipt of the material. When a communication is published the deposited material will be evaluated and included in their files as part of their normal abstracting cycle. The evaluation consists of recalculation of the bond lengths from the author's co-ordinates and comparison of these with the author's values. All data on the Centre's files have to pass this internal consistency test. It will not, however, be possible for the evaluation to be made before the appearance of the preliminary communication in print.
- (iv) Finally, where an author plans not to follow-up his preliminary communication with a full paper he will be required to submit, in addition to the material outlined above, a copy of the structure factor table for the work presented for deposition with the British Library, Lending Division. In this way it too will be available to interested readers.

- (2) In order to aid the readability of communications it is recommended that each should contain a line drawing of the compound under discussion where appropriate.

Papers in Dalton and Perkin Transactions

The sub-committee considered evidence which indicated that X-ray crystallographic papers submitted to the *Journal* were assessed in a less rigorous fashion than those reporting other areas of work. Although the sub-committee felt that this claim was largely unsubstantiated it was agreed that improvement of both assessment procedure and presentation of work was possible. The following recommendations have, therefore, been adopted.

- (1) Crystallographic papers will be assessed for their chemical as well as their crystallographic interest.
- (2) Unless both specifically requested by the author and recommended by the referees for publication, vibrational parameters will be routinely deposited with the structure factors as a Supplementary Publication. Where vibrational parameters are to be published they should be in the form of U_{ij} with units of \AA^2 .
Referees are reminded that they may, at their discretion, recommend other material for deposition where in their view its inclusion in the parent paper is not justified by its interest.
- (3) Each paper should contain a line drawing of the compound under discussion where appropriate in addition to the usual crystallographic figures.

NOTICE TO AUTHORS—No. 12/1977

Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programmes. Many such papers report what would be considered 'routine work' in other areas of chemistry, and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a programme, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

- (i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton, or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.
- (ii) The purpose of the paper and the precise ob-

jectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

- (iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer programme used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.
- (iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

ERRATA

1974, page 1603, right-hand column, line 14: *delete* 'NO⁺' and *insert* 'OH⁻'.

1977, page 1277, Table 5, column 3, entry for compound (19): *delete* '185.4' and *insert* '158.4'.

1978, page 427, left-hand column, first sentence should read: 'Although the chemistry of both silacyclobutanes and compounds containing metal-silicon bonds² is well established, there are few reports^{3a} of silacyclobutanes substituted at silicon by metals'.

page 427, left-hand column, line 10: *delete* ref. 3 and *replace* by ref. 3b.

page 427, left-hand column, references at foot of page: *delete* ref. 3 and *replace* by ³ (a) W. Malisch and M. Kuhn, *Chem. Ber.*, 1974, **107**, 2835; (b) L. E. Gusel'nikov, N. S. Nametkin, and V. M. Vdovin, *Accounts. Chem. Res.*, 1975, **8**, 18.

page 431, left-hand column, line 15: *insert* 'Finally, Malisch and Kuhn^{3a} have characterised the complexes $[M\{\overline{Si(X)CH_2CH_2CH_2}\}]$ [$X = Cl$ or Me and $M = Mo(\eta-C_5H_5)(CO)_3$ or $W(\eta-C_5H_5)(CO)_3$; $X = Cl$ and $M = Fe(\eta-C_5H_5)(CO)_2$; and $X = Me$ and $M = Cr(\eta-C_5H_5)(CO)_3$], obtained from $Cl(X)\overline{SiCH_2CH_2CH_2} + Na[M]$.^{3a}'

page 1728, Table 2: *delete* entries for C(14) and C(15) and *replace* by:

C(14)	0.348(2)	0.735(2)	0.653(2)
C(15)	0.354(1)	0.699(2)	0.736(1)

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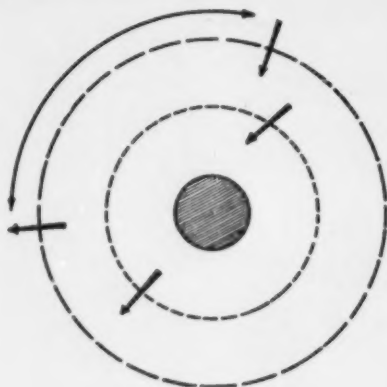
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